

```
18 19 20 21 22 23 24
ring nodes :
    1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
chain bonds :
    7-12 9-19 10-18 16-20 17-21 20-22 21-23
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14
    14-15 15-16 16-17
exact/norm bonds :
    5-7 6-11 7-8 8-9 9-10 10-11 10-18 16-20 17-21 20-22 21-23
exact bonds :
    7-12 9-19
normalized bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17
```

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS

=> d his

(FILE 'HOME' ENTERED AT 15:16:56 ON 20 SEP 2005)

FILE 'REGISTRY' ENTERED AT 15:17:21 ON 20 SEP 2005

L1 STRUCTURE UPLOADED

L2 45 S L1

L3 995 S L1 SSS FUL

FILE 'CAPLUS' ENTERED AT 15:17:51 ON 20 SEP 2005

L4 28 S L3

=> d 11

L1 HAS NO ANSWERS

L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> d ibib abs hitstr total

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10/256,198
```

ANSWER 1 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:673302 CAPLUS

DOCUMENT NUMBER: 143:172909

TITLE: Preparation of tricyclic benzazepines as squalene

synthase inhibitors used for the treatment of

cardiovascular diseases

INVENTOR(S): Woltering, Elisabeth; Haerter, Michael; Flessner,

Timo; Jeske, Mario; Griebenow, Nils; Suessmeier, Frank; Bischoff, Hilmar; Raabe, Martin; Buchmueller, Anja; Kolkhof, Peter; Ellinghaus, Peter; Weber, Olaf

PATENT ASSIGNEE(S): Bayer Healthcare A.-G., Germany

SOURCE:

PCT Int. Appl., 138 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT	KIND DATE				i	APPL	ICAT:	DATE								
	WO 2005	A1 20050728			,	WO 2	004-1		20041231								
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AM,
		ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
•		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,
		MR,	NE,	SN,	TD,	ΤG											
	DE 102004001871						2005	0901		DE 2	004-	1020	0400	1871	20	0040	114
PRIO	RITY APP	LN.	INFO	.:					:	DE 2	004-	1020	0400	1871	A 20	0040	114
GI																	

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB Title compds. I [Z = (CH2)n;n = 1-3; A = aryl, heteroaryl, etc.; X = O, S, NR5; R5 = H, alkyl; Y = N, CR6; R6 = H, OH, alkyl; R1, R2 = H, halo, CN, etc.; R3 = alkyl, alkenyl, alkynyl, etc.; R4 = OR7, NR8R9; R7 = H, alkyl; R8, R9 = H, alkyl, cycloalkyl, etc.] and their pharmaceutically acceptable salts and formulations were prepared For example, condensation of thioamide II and acetyl hydrazine afforded tricyclic benzazepine III in 49% yield. In squalene synthase inhibition assays, compds. I exhibited IC50 values <10 μM.
- IT 860653-00-5P 860653-01-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tricyclic benzazepines as squalene synthase inhibitors used for the treatment of cardiovascular diseases)

RN 860653-00-5 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

10/256,198

$$\begin{array}{c|c} H_2C = CH - CH_2 \\ \hline \\ O & N \\ \hline \\ EtO - C + CH_2 \\ \hline \\ O & N \\ \hline \\ CH_2 & C1 \\ \hline \\ MeO & C1 \\ \hline \end{array}$$

RN 860653-01-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

6

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/256,198

ANSWER 2 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:638758 CAPLUS

DOCUMENT NUMBER: 143:139213

TITLE: Method of improving suitability for granulation

INVENTOR(S): Murakawa, Yusuke; Fukuta, Makoto

PATENT ASSIGNEE(S): Takeda Pharmaceutical Company Limited, Japan

SOURCE: PCT Int. Appl., 27 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.					KIND DATE			1	APPL	ICAT	DATE						
WO 2005065715					A1 20050721				1	WO 2	004-	20041224					
"	W:																
					CU,												
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	zw
	RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
		ΑZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,
		RO,	SE,	SI,	SK,	TR,	BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,
		MR,	ΝE,	SN,	TD,	TG				_					_		

PRIORITY APPLN. INFO.:

JP 2003-430169 A 20031225

AB Disclosed are granules which comprise a compound having poor wettability and a surfactant, especially ones at least about 35 weight% of which do not pass through a Number 100 screen. Also provided is a process for producing granules containing a compound with poor wettability and having improved suitability for granulation, the process comprising adding a surfactant to the compound before or during granulation especially in such an amount that the weight

ratio of the surfactant to the compound is from about 0.001 to about 2.

IT 383652-98-0

RN

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (surfactants for improving granulation of drugs with poor wettability) 383652-98-0 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

REFERENCE COUNT:

26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/256,198

LANGUAGE:

ANSWER 3 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:120907 CAPLUS

DOCUMENT NUMBER: 142:219318

TITLE: Preparation of benzoxazepine derivatives as squalene

synthase inhibitors

INVENTOR(S): Marui, Shogo; Miki, Takashi; Miura, Shoutarou;

Nishimoto, Tomoyuki; Nakada, Yoshihisa Takeda Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 239 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

PATENT ASSIGNEE(S):

Patent Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

P.	ATENT 1	NO.			KIN	D	DATE			APPL:	ICAT:	DATE					
– W	WO 2005012272					A1 20050210			(WO 2	004-	20040730					
	W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
		ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM,	AT,	ΒE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,
		SN,	TD,	ТG													
JP 2005068138						A2 20050317			JP 2004-222658					20040730			730
PRIORITY APPLN. INFO.:									JP 2003-285341						A 2	0030	801
OTHER SOURCE(S):						MARPAT 142:219318											
GI																	

AB The title compds. I (ring A and ring B each represents an optionally substituted benzene ring; ring C represents an optionally further substituted aromatic ring; R1 represents a lower alkyl optionally substituted by optionally substituted hydroxy; X1a represents a bond or optionally substituted lower alkylene; X1b represents a bond or optionally substituted lower alkylene; X2 represents a bond, O, or S; X3 represents a bond or an optionally substituted divalent hydrocarbon group; and Y represents optionally esterified or amidated carboxy) are prepared A

process for preparing I is disclosed. Thus, $(2-[(3R,5S)-7-\text{chloro}-5-(2,3-\text{dimethoxyphenyl})-1-(3-\text{hydroxy}-2,2-\text{dimethylpropyl})-2-\text{oxo}-1,2,3,5-\text{tetrahydro}-4,1-\text{benzoxazepin}-3-yl]methyl]-1,3-\text{thiazol}-5-yl)acetic acid was prepared in a multistep process from 2-(tert-butoxycarbonylamino)acetic acid and potassium monoethyl malonate. Compds. of this invention are said to show IC50 values of <math>\leq 1~\mu\text{M}$ against squalene synthase. Formulations are given.

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IT
     839723-04-5P 839723-05-6P 839723-06-7P
     839723-07-8P 839723-08-9P 839723-09-0P
     839723-10-3P 839723-11-4P 839723-12-5P
    839723-13-6P 839723-14-7P 839723-15-8P
    839723-16-9P 839723-17-0P 839723-18-1P
    839723-19-2P 839723-20-5P 839723-21-6P
     839723-22-7P 839723-23-8P 839723-24-9P
    839723-25-0P 839723-26-1P 839723-27-2P
    839723-28-3P 839723-29-4P 839723-30-7P
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     839723-34-1P 839723-35-2P 839723-36-3P
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     839724-24-2P 839724-25-3P 839724-26-4P
     839724-27-5P 839724-28-6P 839724-29-7P
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     839724-48-0P 839724-49-1P 839724-50-4P
     839725-25-6P 839725-26-7P 839725-27-8P
     839725-28-9P 839725-29-0P 839725-30-3P
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RN

839725-31-4P 839725-32-5P 839725-33-6P 839725-34-7P 839725-35-8P 839725-36-9P 839725-37-0P 839725-38-1P 839725-39-2P 839725-40-5P 839725-41-6P 839725-42-7P 840494-05-5P 840494-06-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzoxazepine derivs. as squalene synthase inhibitors) 839723-04-5 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-05-6 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 839723-06-7 CAPLUS

CN 5-Thiazoleacetic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\alpha$, α -dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-07-8 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-08-9 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-09-0 CAPLUS

CN 5-Thiazolebutanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-10-3 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl](9CI) (CA INDEX NAME)

RN 839723-11-4 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[[1-(hydroxymethyl)cyclobutyl]methyl]-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-12-5 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[[1-(hydroxymethyl)cyclobutyl]methyl]-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-13-6 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-1-propyl-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-14-7 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(2-methylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-(9CI) (CA INDEX NAME)

RN 839723-15-8 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-ethyl-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-16-9 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 839723-17-0 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-18-1 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 839723-19-2 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-20-5 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-methoxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-21-6 CAPLUS

CN 5-Thiazolepropanoic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\beta$ -hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-22-7 CAPLUS

CN 2-Propenoic acid, 3-[2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-thiazolyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 839723-23-8 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-24-9 CAPLUS

CN 4-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-25-0 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-26-1 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-27-2 CAPLUS

CN 4-Thiazolepropanoic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\beta$ -hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-28-3 CAPLUS

CN 2-Propenoic acid, 3-[2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-thiazolyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 839723-29-4 CAPLUS

CN 5-Thiazolecarboxylic acid, 4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-30-7 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, calcium salt (1:1) (9CI) (CA INDEX NAME)

● Ca

RN 839723-31-8 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-methyl-, calcium salt (1:1) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

• Cà

RN 839723-32-9 CAPLUS

CN 5-Oxazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-33-0 CAPLUS

CN 5-Oxazolebutanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-34-1 CAPLUS

CN 5-Oxazoleacetic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\alpha$, α -dimethyl- (9CI) (CA INDEX NAME)

RN 839723-35-2 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-36-3 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-(9CI) (CA INDEX NAME)

RN 839723-37-4 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(2-methylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-38-5 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-1-propyl-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-39-6 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-ethyl-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-40-9 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 839723-41-0 CAPLUS

CN 4-Oxazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-42-1 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-43-2 CAPLUS

CN 1H-Pyrazole-1-butanoic acid, 4-carboxy-3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-44-3 CAPLUS

CN 1H-Pyrazole-1-butanoic acid, 4-carboxy-5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-45-4 CAPLUS

CN 1H-Pyrazole-1-acetic acid, 4-carboxy-3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-46-5 CAPLUS

CN 1H-Pyrazole-1-acetic acid, 4-carboxy-5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-47-6 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1-(2-carboxyphenyl)-, 4-ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-48-7 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1-(3-carboxyphenyl)-, 4-ethyl ester (9CI) (CA INDEX NAME)

RN 839723-49-8 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1-(4-carboxyphenyl)-, 4-ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-50-1 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(2-carboxyphenyl)-5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-51-2 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(3-carboxyphenyl)-5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-52-3 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-(4-carboxyphenyl)-5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-53-4 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-54-5 CAPLUS

CN 2-Propenoic acid, 3-[1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-1H-pyrazol-5-yl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839723-55-6 CAPLUS

CN 1H-Imidazole-5-carboxylic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-56-7 CAPLUS

CN 1H-Pyrrole-2-carboxylic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

RN 839723-57-8 CAPLUS

CN 1,3,4-Oxadiazole-2-acetic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-58-9 CAPLUS

CN 1,3,4-Thiadiazole-2-acetic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-59-0 CAPLUS

CN 1,3,4-Thiadiazole-2-propanoic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-60-3 CAPLUS

CN 1,2,4-Oxadiazole-4(5H)-acetic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-oxo- (9CI) (CA INDEX NAME)

RN 839723-61-4 CAPLUS

CN 1,2,4-Oxadiazole-4(5H)-acetic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-oxo-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-62-5 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-63-6 CAPLUS

CN 1,2,4-Oxadiazole-5-acetic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-64-7 CAPLUS

CN 1H-1,2,4-Triazole-3-carboxylic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-65-8 CAPLUS

CN 1H-1,2,4-Triazole-3-acetic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

.Absolute stereochemistry.

RN 839723-66-9 CAPLUS

CN Benzoic acid, 3-[3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-hydroxy-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

RN 839723-67-0 CAPLUS

CN Benzoic acid, 3-[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-hydroxy-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-68-1 CAPLUS

CN Benzoic acid, 4-[3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-hydroxy-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

RN 839723-69-2 CAPLUS

CN Benzoic acid, 4-[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-hydroxy-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-70-5 CAPLUS

CN Benzoic acid, 4-[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-ethoxy-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)

RN 839723-71-6 CAPLUS

CN 1H-Pyrazole-1-acetic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-72-7 CAPLUS

CN 1H-Pyrazole-1-acetic acid, 5-(carboxymethoxy)-3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-73-8 CAPLUS

CN 2-Propenoic acid, 3-[4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839723-74-9 CAPLUS

CN Benzenepropanoic acid, 4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 839723-75-0 CAPLUS

CN 2-Propenoic acid, 3-[4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 839723-76-1 CAPLUS

CN 2-Propenoic acid, 3-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

$$MeO$$
 MeO
 MeO
 MeO
 MeO
 R
 $C1$
 $CMe3$

RN 839723-77-2 CAPLUS

CN 2-Propenoic acid, 3-[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839723-78-3 CAPLUS

CN Benzenepropanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 839723-79-4 CAPLUS

CN Benzenepropanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$MeO$$
 MeO
 MeO
 R
 R
 $CMe3$

RN 839723-80-7 CAPLUS

CN Benzenepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

RN 839723-81-8 CAPLUS

CN Benzenebutanoic acid, 4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-82-9 CAPLUS

CN Benzenepropanoic acid, 4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]-1-hydroxyethyl]- (9CI) (CA INDEX NAME)

RN 839723-83-0 CAPLUS

CN Benzenepropanoic acid, 4-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-84-1 CAPLUS

CN Benzoic acid, 4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 839723-85-2 CAPLUS

CN Benzoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-86-3 CAPLUS

CN Acetic acid, [4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]phenoxy]- (9CI) (CA INDEX NAME)

RN 839723-87-4 CAPLUS

CN Benzeneacetic acid, 4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-88-5 CAPLUS

CN 3-Furancarboxylic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839723-89-6 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-90-9 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-(2-phenylethyl)- (9CI) (CA INDEX NAME)

RN 839723-91-0 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-(2-phenylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-92-1 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

RN 839723-93-2 CAPLUS

CN 1H-Pyrazole-5-propanoic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-94-3 CAPLUS

CN 1H-Pyrazole-4-propanoic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

RN 839723-95-4 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-[2-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-96-5 CAPLUS

CN 1H-Pyrazole-3-propanoic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-β-hydroxy- (9CI) (CA INDEX NAME)

RN 839723-97-6 CAPLUS

CN 1H-Pyrazole-5-propanoic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-β-hydroxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839723-98-7 CAPLUS

CN 2-Propenoic acid, 3-[1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-1H-pyrazol-4-yl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839723-99-8 CAPLUS

CN 1,3,4-Thiadiazole-2-butanoic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-00-4 CAPLUS

CN 5-Thiazoleacetic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\alpha$ -(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 839724-01-5 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-02-6 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, calcium salt (2:1) (9CI) (CA INDEX NAME)

●1/2 Ca

RN 839724-03-7 CAPLUS

CN 5-Thiazoleacetic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\alpha$ -(phenylmethylene)-, (α Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 839724-04-8 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-\(\alpha\)-hydroxy-, (\(\alpha\)R) - (9CI) (CA INDEX NAME)

RN 839724-05-9 CAPLUS

CN 4-Thiazolepropanoic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\beta$, β -dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-06-0 CAPLUS

CN 5-Thiazoleacetic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

RN 839724-07-1 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-08-2 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

RN 839724-09-3 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-10-6 CAPLUS

CN 4-Thiazoleacetic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

RN 839724-11-7 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[2-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-12-8 CAPLUS

CN 4-Thiazolepropanoic acid, $2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-<math>\beta$ -hydroxy- (9CI) (CA INDEX NAME)

RN 839724-13-9 CAPLUS

CN 2-Propenoic acid, 3-[2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-4-thiazolyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 839724-14-0 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

RN 839724-15-1 CAPLUS

CN 4-Thiazolepropanoic acid, $2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-<math>\beta$, β -dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-16-2 CAPLUS

CN 4-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 839724-17-3 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-18-4 CAPLUS

CN 4-Thiazoleacetic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]-1-hydroxyethyl]- (9CI) (CA INDEX NAME)

RN 839724-19-5 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]-1-hydroxyethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-20-8 CAPLUS

CN 2-Thiopheneacetic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 839724-21-9 CAPLUS

CN 5-Thiazolecarboxylic acid, 4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-22-0 CAPLUS

CN 5-Thiazoleacetic acid, 2-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (9CI) (CA INDEX NAME)

RN 839724-23-1 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-24-2 CAPLUS

CN 4-Thiazoleacetic acid, 2-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (9CI) (CA INDEX NAME)

RN 839724-25-3 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-26-4 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 839724-27-5 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-28-6 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839724-29-7 CAPLUS

CN 4-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-30-0 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-methyl- (9CI) (CA INDEX NAME)

RN 839724-31-1 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-32-2 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-(9CI) (CA INDEX NAME)

RN 839724-33-3 CAPLUS

CN 5-Oxazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-34-4 CAPLUS

CN 4-Oxazolepropanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-methyl- (9CI) (CA INDEX NAME)

RN 839724-35-5 CAPLUS

CN 1,2,4-Oxadiazole-5-butanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-36-6 CAPLUS

CN 1,2,4-Oxadiazole-5-pentanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839724-37-7 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-38-8 CAPLUS

CN 1,2,4-Oxadiazole-5-butanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

$$Me_3C$$
 ON
 R
 $C1$
 MeO
 OMe

RN 839724-39-9 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-40-2 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

RN 839724-41-3 CAPLUS

CN 1,2,4-Oxadiazole-5-butanoic acid, 3-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-42-4 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (9CI) (CA INDEX NAME)

$$Me_3C$$

ON

 $(CH_2)_3$

R

 R
 OMe

OMe

RN 839724-43-5 CAPLUS

CN 1,2,4-Oxadiazole-5-butanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- β -methyl-, (β R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-44-6 CAPLUS

CN Acetic acid, [[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-oxadiazol-5-yl]methyl]thio]- (9CI) (CA INDEX NAME)

RN 839724-45-7 CAPLUS

CN Propanoic acid, 2-[[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-oxadiazol-5-yl]methyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-46-8 CAPLUS

CN Acetic acid, [[1-[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-oxadiazol-5-yl]-1-methylethyl]thio]- (9CI) (CA INDEX NAME)

RN

839724-47-9 CAPLUS Acetic acid, [[1-[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-CN tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3yl]methyl]-1,2,4-oxadiazol-5-yl]-1-methylethyl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN839724-48-0 CAPLUS

Acetic acid, [[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-CN tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3yl]methyl]-1,2,4-oxadiazol-5-yl]methyl]thio]- (9CI) (CA INDEX NAME)

RN 839724-49-1 CAPLUS

CN Propanoic acid, 2-[[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-oxadiazol-5-yl]methyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-50-4 CAPLUS

CN Acetic acid, [[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-thiadiazol-5-yl]thio]- (9CI) (CA INDEX NAME)

RN 839725-25-6 CAPLUS

CN Propanoic acid, 2-[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-thiadiazol-5-yl]thio]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-26-7 CAPLUS

CN Butanoic acid, 4-[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-thiadiazol-5-yl]thio]- (9CI) (CA INDEX NAME)

RN

839725-27-8 CAPLUS Acetic acid, [[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-CNtetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3yl]methyl]-1,2,4-thiadiazol-5-yl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN839725-28-9 CAPLUS

CN 1,2,4-Oxadiazole-5-pentanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839725-29-0 CAPLUS

CN 1,2,4-Oxadiazole-5-butanoic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-30-3 CAPLUS

CN 1,2,4-Oxadiazole-5-pentanoic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839725-31-4 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-32-5 CAPLUS

CN 1,2,4-Oxadiazole-5-butanoic acid, 3-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (9CI) (CA INDEX NAME)

HO₂C
$$(CH_2)_3$$
 $(CH_2)_3$ $(C$

RN 839725-33-6 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-34-7 CAPLUS

CN 5-Thiazolebutanoic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

RN 839725-35-8 CAPLUS

CN 5-Thiazolebutanoic acid, 2-[3-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-36-9 CAPLUS

CN 1,3,4-Oxadiazole-2-butanoic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839725-37-0 CAPLUS

CN 1,3,4-Oxadiazole-2-propanoic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-38-1 CAPLUS

CN 5-Thiazolepropanoic acid, $4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\beta$ -hydroxy- (9CI) (CA INDEX NAME)

RN 839725-39-2 CAPLUS

CN 2-Propenoic acid, 3-[4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-thiazolyl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 839725-40-5 CAPLUS

CN 5-Thiazolepropanoic acid, 4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839725-41-6 CAPLUS

CN 5-Thiazolebutanoic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$Me$$
 Me Me HO R S $C1$ MeO OMe

RN 839725-42-7 CAPLUS

CN 2-Thiophenebutanoic acid, 5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 840494-05-5 CAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 1-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 840494-06-6 CAPLUS

CN Benzenepropanoic acid, 4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

IT 171868-39-6 383661-55-0 839725-20-1 839725-23-4 839725-24-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of benzoxazepine derivs. as squalene synthase inhibitors)

RN 171868-39-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383661-55-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 839725-20-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetonitrile, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-23-4 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-3-[[5-(chloromethyl)-1,2,4-oxadiazol-3-yl]methyl]-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,5-dihydro-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 839725-24-5 CAPLUS

CN 4,1-Benzoxazepine-3-ethanethioamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)-(9CI) (CA INDEX NAME)

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IT
    189059-52-7P 839724-51-5P 839724-52-6P
     839724-54-8P 839724-55-9P 839724-56-0P
    839724-57-1P 839724-58-2P 839724-59-3P
     839724-60-6P 839724-61-7P 839724-62-8P
     839724-63-9P 839724-64-0P 839724-65-1P
     839724-66-2P 839724-67-3P 839724-68-4P
     839724-69-5P 839724-70-8P 839724-71-9P
     839724-72-0P 839724-73-1P 839724-74-2P
     839724-75-3P 839724-76-4P 839724-77-5P
     839724-78-6P 839724-79-7P 839724-80-0P
     839724-81-1P 839724-82-2P 839724-83-3P
     839724-84-4P 839724-85-5P 839724-86-6P
     839724-87-7P 839724-88-8P 839724-89-9P
     839724-90-2P 839724-91-3P 839724-92-4P
     839724-93-5P 839724-94-6P 839724-95-7P
     839724-96-8P 839724-97-9P 839724-98-0P
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RN

CN

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839724-99-1P 839725-00-7P 839725-01-8P
839725-02-9P 839725-03-0P 839725-04-1P
839725-05-2P 839725-06-3P 839725-07-4P
839725-08-5P 839725-09-6P 839725-10-9P
839725-11-0P 839725-12-1P 839725-13-2P
839725-14-3P 839725-15-4P 839725-16-5P
839725-17-6P 839725-43-8P 839725-44-9P
839725-45-0P 839725-46-1P 839725-47-2P
839725-48-3P 839725-49-4P 841236-35-9P
841236-36-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
   (preparation of benzoxazepine derivs. as squalene synthase inhibitors)
189059-52-7 CAPLUS
4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-
dimethylpropy1)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)
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Absolute stereochemistry.

RN 839724-51-5 CAPLUS
CN Butanoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3yl]acetyl]amino]-4-oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 839724-52-6 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-54-8 CAPLUS

CN Pentanoic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 839724-55-9 CAPLUS

CN 4,1-Benzoxazepine-3-ethanethioic acid, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-56-0 CAPLUS

CN Butanoic acid, 2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]thio]-3-oxo-, methyl ester (9CI) (CA INDEX NAME)

RN 839724-57-1 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-methyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-58-2 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 839724-59-3 CAPLUS

CN 4,1-Benzoxazepine-3-ethanethioamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-60-6 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 839724-61-7 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

.Absolute stereochemistry.

RN 839724-62-8 CAPLUS

CN 5-Thiazolepropanoic acid, $2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\beta$ -oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 839724-63-9 CAPLUS

CN 5-Thiazolepropanoic acid, $2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\beta$ -hydroxy-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-64-0 CAPLUS

CN 2-Propenoic acid, 3-[2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-thiazolyl]-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 839724-65-1 CAPLUS

CN Hexanoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-5-oxo-, methyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-66-2 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-methyl-, methyl ester (9CI) (CA INDEX NAME)

RN 839724-67-3 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-68-4 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 839724-69-5 CAPLUS

CN 4,1-Benzoxazepine-3-butanoic acid, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro- β ,2-dioxo-, ethyl ester, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-70-8 CAPLUS

CN 5-Thiazolecarboxylic acid, 4-[((3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 839724-71-9 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-72-0 CAPLUS

CN 5-Oxazoleacetic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839724-73-1 CAPLUS

CN 5-Oxazolepropanoic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-74-2 CAPLUS

CN 4-Oxazolepropanoic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-methyl-, methyl ester (9CI) (CA INDEX NAME)

RN 839724-75-3 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

.Absolute stereochemistry.

RN 839724-76-4 CAPLUS

CN 1H-Pyrazole-1-butanoic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-4-(ethoxycarbonyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 839724-77-5 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-3-(2-hydroxyethyl)-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-78-6 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 1-[2-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 839724-79-7 CAPLUS

CN 1H-Pyrazole-3-acetic acid, 1-[2-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-80-0 CAPLUS

CN Propanedioic acid, monoethyl ester, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]hydrazide (9CI) (CA INDEX NAME)

RN 839724-81-1 CAPLUS

CN 1,3,4-Oxadiazole-2-acetic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-82-2 CAPLUS

CN 1,3,4-Thiadiazole-2-acetic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 839724-83-3 CAPLUS

CN Butanedioic acid, monoethyl ester, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-84-4 CAPLUS

CN 1,3,4-Thiadiazole-2-propanoic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 839724-85-5 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-3-[(2,5-dihydro-5-oxo-1,2,4-oxadiazol-3-yl)methyl]-5-(2,3-dimethoxyphenyl)-1,5-dihydro-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-86-6 CAPLUS

CN 1,2,4-Oxadiazole-4(5H)-acetic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-oxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 839724-87-7 CAPLUS

CN Benzoic acid, 4-[3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-ethoxy-1H-pyrazol-1-yl]-, ethyl ester (9CI) (CA INDEX NAME)

.Absolute stereochemistry.

RN 839724-88-8 CAPLUS

CN Benzoic acid, 4-[3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-5-hydroxy-1H-pyrazol-1-yl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 839724-89-9 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 3-[2-(4-bromophenyl)-2-oxoethyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-1-(3-hydroxy-2,2-dimethylpropyl)-, (3R,5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-90-2 CAPLUS

CN 2-Propenoic acid, 3-[4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]phenyl]-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 839724-91-3 CAPLUS

CN Benzenepropanoic acid, 4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-92-4 CAPLUS

CN Benzenepropanoic acid, 4-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 839724-93-5 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-1-(3-hydroxy-2,2-dimethylpropyl)-3-[2-(4-hydroxyphenyl)-2-oxoethyl]-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-94-6 CAPLUS

CN Benzeneacetic acid, 4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 839724-95-7 CAPLUS

CN 4-Thiazolepropanoic acid, 2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-96-8 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,2-dimethylpropyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 839724-97-9 CAPLUS

CN 5-Thiazoleacetic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[3-[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,2-dimethylpropyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\alpha$ -(phenylmethyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839724-98-0 CAPLUS

CN 5-Thiazoleacetic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\alpha$ -(phenylmethyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 839724-99-1 CAPLUS

CN 5-Thiazoleacetic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[3-[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,2-dimethylpropyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\alpha$ - (hydroxyphenylmethyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-00-7 CAPLUS

CN 5-Thiazoleacetic acid, $2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[3-[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,2-dimethylpropyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-<math>\alpha$ -(phenylmethylene)-, ethyl ester, (α Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 839725-01-8 CAPLUS

CN 4,1-Benzoxazepine-3-propanenitrile, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-02-9 CAPLUS

CN 4,1-Benzoxazepine-3-propanethioamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 839725-03-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetaldehyde, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-04-1 CAPLUS

CN 4-Thiazolepropanenitrile, $2-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-<math>\alpha-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-(9CI)$ (CA INDEX NAME)

RN 839725-05-2 CAPLUS

CN 4,1-Benzoxazepine-3-propanethioamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)- α -[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-06-3 CAPLUS

CN 4-Thiazoleacetic acid, 2-[2-[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]-1-hydroxyethyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 839725-07-4 CAPLUS

CN 4-Thiazoleacetic acid, 2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-08-5 CAPLUS

CN 2-Butenoic acid, 4-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]-, ethyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 839725-09-6 CAPLUS

CN 4,1-Benzoxazepine-3-butanoic acid, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-10-9 CAPLUS

CN 4,1-Benzoxazepine-3-butanenitrile, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 839725-11-0 CAPLUS

CN 4,1-Benzoxazepine-3-butanethioamide, 1-[2-(acetyloxy)-2-methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-12-1 CAPLUS

CN 1,2,4-Oxadiazole-5-acetonitrile, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]- (9CI) (CA INDEX NAME)

RN 839725-13-2 CAPLUS

CN 4,1-Benzoxazepine-3-ethanimidamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-hydroxy-2-oxo-, (3R,5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-14-3 CAPLUS

CN 1,2,4-Oxadiazole-5-pentanoic acid, 3-[[(3R,5s)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Me 3 C
$$(CH_2)$$
 4 N R $C1$ MeO MeO OMe

RN 839725-15-4 CAPLUS

CN Ethanethioic acid, O-[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-oxadiazol-5-yl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-16-5 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-3-[(5-chloro-1,2,4-thiadiazol-3-yl)methyl]-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,5-dihydro-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 839725-17-6 CAPLUS

CN Acetic acid, [[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-thiadiazol-5-yl]thio]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-43-8 CAPLUS

CN Propanoic acid, 2-[[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-1,2,4-thiadiazol-5-yl]thio]-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 839725-44-9 CAPLUS

CN 1,2,4-Oxadiazole-5-pentanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-45-0 CAPLUS

CN 2-Butenenitrile, 4-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]-, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 839725-46-1 CAPLUS

CN 4,1-Benzoxazepine-3-butanimidamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-N-hydroxy-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-47-2 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[2-[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]-1-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 839725-48-3 CAPLUS

CN 1,2,4-Oxadiazole-5-propanoic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 839725-49-4 CAPLUS

CN 1,3,4-Oxadiazole-2-propanoic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 841236-35-9 CAPLUS

CN 4,1-Benzoxazepine-3-ethanimidamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-N-hydroxy-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 841236-36-0 CAPLUS

CN 4,1-Benzoxazepine-3-propanimidamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)- α -[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1,2,3,5-tetrahydro-N-hydroxy-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN A¢CESSION NUMBER: 2004:902194 CAPLUS DOCUMENT NUMBER: 141:395590 TITLE: Preparation of benzoxazepine compounds as RFRP receptor antagonists INVENTOR(S): Itoh, Fumio; Hinuma, Shuji; Kanzaki, Naoyuki; Mabuchi, Hiroshi; Yoshida, Hiromi; Matsumoto, Hirokazu; Wakabayashi, Takeshi Takeda Chemical Industries Ltd., Japan PATENT ASSIGNEE(S): PCT Int. Appl., 226 pp. SOURCE: CODEN: PIXXD2 DOCUMENT TYPE: Patent Japanese LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE -----WO 2004-JP5406 **⊋**0041028 WO 2004091628 A1 20040415 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG JP 2004331659 A2 20041125 JP 2004-120246 20040415 PRIORITY APPLN. INFO.: JP 2003-114313 A 20030418 OTHER SOURCE(S): MARPAT 141:395590 GΙ * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT * Title compds. I [A = (un)substituted aromatic ring; B = (un)substituted AB benzene ring; X = 0, S(:0)n, NR3; n = 0-2; R3 = H, (un)substituted hydrocarbon group, etc.; R1, R2 = H, (un) substituted hydrocarbon group, etc.] were prepared For example, reductive amination of compound trans-II·HCl [Q = H] with 3-phenylpropanaldehyde afforded compound trans-II·HCl [Q = 3-phenylpropyl]. In human RFRP-3

(RFamide-related peptide-3) binding inhibition assays, the IC50 value was <1 µM. Compds. I are claimed useful as analgesics, prolactin secretion regulators, etc. Formulations are given.

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TΤ
     782466-03-9P 782466-05-1P 782466-07-3P
     782466-49-3P 782466-51-7P 782466-55-1P
     782466-61-9P 782466-67-5P 782466-69-7P
     782466-71-1P 782466-75-5P 782466-77-7P
     782467-32-7P 782467-34-9P 782467-38-3P
     782467-40-7P 782467-45-2P 782467-51-0P,
     trans-[7-Chloro-1-(2,2-dimethylpropyl)-5-(2-methoxy-3-[3-[methyl(3-
     phenylpropyl)amino]propoxy]phenyl)-2-oxo-1,2,3,5-tetrahydro-4,1-
     benzoxazepin-3-yl]acetic acid ethyl ester hydrochloride
```

Relative stereochemistry.

t-BuO
$$MeO$$
 MeO MeO R CMe_3

RN 782466-05-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 5-[3-(3-aminopropoxy)-2-methoxyphenyl]-7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782466-07-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-

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(9CI) (CA INDEX NAME)

Relative stereochemistry.

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

HCl

RN 782466-49-3 CAPLUS

CN Carbamic acid, [2-[3-[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-3-[2-[[(2-fluorophenyl)methyl]amino]-2-oxoethyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-5-yl]-2-methoxyphenoxy]ethyl]-, 1,1-dimethylethyl ester, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782466-51-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 5-[3-(2-aminoethoxy)-2-methoxyphenyl]-7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

$$H_2N$$
 MeO
 R
 CMe_3

HCl

RN 782466-55-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[2-[(3-phenylpropyl)amino]ethoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782466-61-9 CAPLUS

CN Carbamic acid, [3-[3-[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-3-[2-[[(2-fluorophenyl)methyl]amino]-2-oxoethyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-5-yl]-2-methoxyphenoxy]propyl](3-phenylpropyl)-,
1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

RN 782466-67-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-[3-[3-[[(1,1-dimethylethoxy)carbonyl]amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782466-69-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 5-[3-(3-aminopropoxy)-2-methoxyphenyl]-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

HC1

RN 782466-71-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, ethyl ester, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Meo
$$C1$$
 $C1$
 $CH_2)_3$
 $CH_2)_3$
 $CH_2)_3$
 $CH_2)_3$

● HCl

RN 782466-75-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-[3-[3-[[(1,1-dimethylethoxy)carbonyl](3-phenylpropyl)amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782466-77-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-[3-[3-[(1,1-dimethylethoxy)carbonyl](3-phenylpropyl)amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782467-32-7 CAPLUS

CN Carbamic acid, [3-[3-[(3R,5S)-7-chloro-1-[(2,4-dimethoxyphenyl)methyl]-3-[2-[((2-fluorophenyl)methyl]amino]-2-oxoethyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-5-yl]-2-methoxyphenoxy]propyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

RN 782467-34-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 5-[3-(3-aminopropoxy)-2-methoxyphenyl]-7-chloro-1-[(2,4-dimethoxyphenyl)methyl]-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782467-38-3 CAPLUS

CN Carbamic acid, [3-[3-[(3R,5S)-7-chloro-3-[2-[[(2-fluorophenyl)methyl]amino]-2-oxoethyl]-1,2,3,5-tetrahydro-1-methyl-2-oxo-4,1-benzoxazepin-5-yl]-2-methoxyphenoxy]propyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782467-40-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 5-[3-(3-aminopropoxy)-2-methoxyphenyl]-7-chloro-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-1-methyl-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

$$H_2N$$
 (CH_2)
 3
 MeO
 R
 N
 H
 N
 Me
 N
 Me

● HCl

RN 782467-45-2 CAPLUS

CN 4,1-Benzoxazepine-1,3(5H)-diacetic acid, 7-chloro-2,3-dihydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, α1-(1,1-dimethylethyl) α3-methyl ester, (3R,5S)-rel-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 782467-44-1 CMF C37 H45 C1 N2 O8

$$t-BuO$$

NeO

R

S

C1

 $(CH_2)_3$
 $(CH_2)_3$

Ph

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 782467-51-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[methyl(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, ethyl ester, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

● HCl

RN 782467-55-4 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-[3-[3-[3-(2-chlorophenyl)propyl]amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

Meo C1
$$(CH_2)_3$$
 $(CH_2)_3$ $(CH_2)_3$ $(CH_2)_3$

● HCl

RN 782467-57-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-[3-[3-[3-(2-chlorophenyl)propyl][(1,1-dimethylethoxy)carbonyl]amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl

ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782467-59-8 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-[3-[3-[3-(2-chlorophenyl)propyl][(1,1-dimethylethoxy)carbonyl]amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782467-65-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-[3-[3-[3-[3-(2-chlorophenyl)propyl]methylamino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

RN 782467-67-8 CAPLUS
CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-[3-[3-[3-[3-(2-chlorophenyl)propyl]methylamino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782467-71-4 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, 4-piperidinyl ester, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX

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NAME)

Relative stereochemistry.

Ph
$$(CH_2)$$
 3 (CH_2) 3

● HCl

RN 782468-11-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

RN 782468-62-6 CAPLUS

CN 2-Piperazinecarboxylic acid, 4-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, rel- (9CI) (CA INDEX NAME)

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

RN 782469-59-4 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[methyl(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

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TT 782466-09-5P 782466-11-9P 782466-13-1P 782466-15-3P 782466-17-5P 782466-19-7P 782466-21-1P 782466-23-3P 782466-25-5P 782466-27-7P 782466-29-9P 782466-31-3P 782466-33-5P 782466-35-7P 782466-37-9P 782466-39-1P 782466-41-5P 782466-43-7P 782466-45-9P 782466-47-1P 782466-53-9P 782466-57-3P 782466-59-5P 782466-73-3P 782466-79-9P 782466-81-3P 782466-83-5P 782466-85-7P 782466-87-9P 782466-99-1P 782466-91-5P 782466-93-7P 782466-95-9P 782466-97-1P 782466-99-3P 782467-01-0P
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     782467-15-6P 782467-17-8P 782467-19-0P
     782467-21-4P 782467-23-6P 782467-25-8P
     782467-28-1P 782467-30-5P 782467-36-1P
     782467-42-9P 782467-47-4P 782467-53-2P
     782467-61-2P 782467-63-4P 782467-69-0P
     782467-73-6P 782467-75-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of benzoxazepine compds. as agents for controlling function of
        RFRP receptor)
     782466-09-5 CAPLUS
RN
CN
     4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-
     fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-
     (pentylamino)propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI)
       (CA INDEX NAME)
```

Me (CH₂)
$$\frac{H}{4}$$
 (CH₂) $\frac{1}{3}$ 0 MeO CMe₃

HCl

```
RN 782466-11-9 CAPLUS
CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(phenylmethyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)
```

• HC1

RN 782466-13-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-5-[3-[3-[(2-furanylmethyl)amino]propoxy]-2-methoxyphenyl]-1,2,3,5-tetrahydro-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782466-15-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(2-thienylmethyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

$$Me3C$$
 R
 S
 $C1$
 H
 $C1$
 $CH_2)_3$
 H
 S

HCl

RN 782466-17-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(2-pyridinylmethyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782466-19-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(2-naphthalenylmethyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride,

HCl

RN 782466-21-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(1-naphthalenylmethyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

HCl

RN 782466-23-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-

fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(4-phenylbutyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

HCl

RN 782466-25-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-[3-[3-[3-(4-chlorophenyl)propyl]amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782466-27-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-[3-[3-[3-[3-(3-chlorophenyl)propyl]amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782466-29-9 CAPLUS
CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-[3-[3-[[3-(2-chlorophenyl)propyl]amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

HCl

RN 782466-31-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[methyl(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782466-33-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(2-phenoxyethyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-

10/256,198

(9CI) (CA INDEX NAME)

Relative stereochemistry.

HCl

RN 782466-35-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(2-phenylethyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

● HCl

RN 782466-37-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[[(2E)-3-phenyl-2-propenyl]amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-

(9CI) (CA INDEX NAME)

Relative stereochemistry. Double bond geometry as shown.

HCl

RN 782466-39-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[[3-(4-methoxyphenyl)propyl]amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

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__OMe

RN 782466-41-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[[3-(3-methoxyphenyl)propyl]amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

● HCl

_ OMe

RN 782466-43-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[[3-(2-methoxyphenyl)propyl]amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Me 3 C
$$R$$
 $C1$ R $C1$ R $CH_2)_3$ R $CH_2)_3$ R $CH_2)_3$ R $CH_2)_3$ R $CH_2)_3$

● HCl

RN 782466-45-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-[3-[3-[3-(3,4-dimethoxyphenyl)propyl]amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

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● HCl

PAGE 1-B

__OMe

RN 782466-47-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[3-[3-[[2-(1H-indol-3-yl)ethyl]amino]propoxy]-2-methoxyphenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

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PAGE 1-B

● HCl

RN 782466-53-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[2-[(2-phenylethyl)amino]ethoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

RN 782466-57-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[2-[(4-phenylbutyl)amino]ethoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782466-59-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[2-[methyl(3-phenylpropyl)amino]ethoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

HCl

RN 782466-73-3 CAPLUS
CN 4,1-Benzoxazepine-3-acetic acid, 5-[3-[3-[bis(3-phenylpropyl)amino]propoxy]-2-methoxyphenyl]-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782466-79-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

RN 782466-81-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Meo
$$C1$$

Meo $C1$

Meo $C1$

Meo $C1$
 $C1$

HCl

RN 782466-83-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-N-(phenylmethyl)-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me}_3\text{C} \\ \text{Ph} \\ \text{N} \\ \text{Me}_0 \\ \text{CCH}_2)_3 \end{array} \begin{array}{c} \text{C} \\ \text{CH}_2)_3 \end{array} \begin{array}{c} \text{Ph} \\ \text{CH}_2)_3 \end{array}$$

RN 782466-85-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-N-(2-phenylethyl)-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Ph
$$\frac{N}{H}$$
 $\frac{N}{C1}$ $\frac{N}{C1$

HCl

RN 782466-87-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-N-methyl-2-oxo-N-(phenylmethyl)-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Ph N S Cl MeO
$$(CH_2)_3$$
 $(CH_2)_3$ $(CH_2)_3$

RN 782466-89-1 CAPLUS

.CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-N-phenyl-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782466-91-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-N-(2-pyridinylmethyl)-, dihydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

●2 HCl

RN 782466-93-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-N-propyl-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782466-95-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N,N-diethyl-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

$$Me3C$$
 R
 S
 $C1$
 $C1$
 $CH_2)_3$
 $CH_2)_3$
 $CH_2)_3$

HCl

RN 782466-97-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-[(2-methoxyphenyl)methyl]-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782466-99-3 CAPLUS

CN Piperidine, 1-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

HCl

RN 782467-01-0 CAPLUS

CN Piperazine, 1-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, dihydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

•2 HCl

RN 782467-03-2 CAPLUS

CN Piperazine, 1-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-methyl-, dihydrochloride, rel- (9CI) (CA INDEX NAME)

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

RN 782467-05-4 CAPLUS

CN Morpholine, 4-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

● HCl

RN 782467-07-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-N-(4-piperidinylmethyl)-, dihydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

RN 782467-09-8 CAPLUS

CN 1,4'-Bipiperidine, 1'-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, dihydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

●2 HCl

RN 782467-11-2 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, N-(2-aminoethyl)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, dihydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

$$H_2N$$
 H_2N
 H_2N
 H_3C
 R
 $C1$
 $C1$
 $CH_2)_3$
 $CH_2)_3$

●2 HCl

RN 782467-13-4 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, N-(3-aminopropyl)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, dihydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

$$Me_3C$$
 $(CH_2)_3$
 N
 H_2N
 $(CH_2)_3$
 $(CH_2)_3$
 $(CH_2)_3$
 $(CH_2)_3$
 $(CH_2)_3$

●2 HC1

RN 782467-15-6 CAPLUS

CN 4-Piperidinamine, 1-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-

4,1-benzoxazepin-3-yl]acetyl]-, dihydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

●2 HCl

RN 782467-17-8 CAPLUS

CN 1H-1,4-Diazepine, 1-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]hexahydro-, dihydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

●2 HCl

RN 782467-19-0 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-1-(2,2-dimethylpropyl)-1,5-dihydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-3-[2-oxo-2-(4-piperidinyl)ethyl]-, dihydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

●2 HCl

RN 782467-21-4 CAPLUS

CN Glycine, N-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782467-23-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-[3-[3-(dimethylamino)propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

● HCl

RN 782467-25-8 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[2-(1-pyrrolidinyl)ethoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782467-28-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-(4-methyl-1-piperazinyl)propoxy]phenyl]-2-oxo-, dihydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

●2 HCl

RN 782467-30-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-[3-[2-(dimethylamino)ethoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

HCl

RN 782467-36-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-[(2,4-dimethoxyphenyl)methyl]-N[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, monohydrochloride, (3R,5S)-rel(9CI) (CA INDEX NAME)

RN 782467-42-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-1-methyl-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 782467-47-4 CAPLUS

CN 4,1-Benzoxazepine-1,3(5H)-diacetic acid, 7-chloro-2,3-dihydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, α3-methyl ester, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

● HCl

RN 782467-53-2 CAPLUS

CN Piperazine, 1-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[methyl(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, dihydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

●2 HCl

RN 782467-61-2 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-[3-[3-[3-(2-chlorophenyl)propyl]amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, monohydrochloride, (3R,5S)-rel- (9CI) (CA INDEX NAME)

● HCl

RN 782467-63-4 CAPLUS

CN Piperazine, 1-[[(3R,5S)-7-chloro-5-[3-[3-[[3-(2-chlorophenyl)propyl]amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, dihydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Meo
$$C1$$

Meo $C1$
 $C1$
 $CH_2)_3$
 $C1$
 $CH_2)_3$

●2 HCl

RN 782467-69-0 CAPLUS

CN Piperazine, 1-[[(3R,5S)-7-chloro-5-[3-[3-[(3-(2-chlorophenyl)propyl]methylamino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, dihydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

●2 HCl

RN 782467-73-6 CAPLUS
CN 4-Piperidinol, 1-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

HCl

RN 782467-75-8 CAPLUS

CN 2-Piperazinecarboxylic acid, 4-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, dihydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

●2 HCl

Ph
$$(CH_2)_5$$
 $(CH_2)_3$ $(CH_2)_3$ $(CH_2)_4$ $(CH_2)_5$ (CH_2)

RN 782469-00-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[[(2E)-3-phenyl-2-propenyl]amino]propoxy]phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

$$\begin{array}{c|c} Ph & E & H \\ N & (CH_2)_3 & \\ \hline MeO & S & C1 \\ \hline M & N & CMe_3 \\ \end{array}$$

RN 782469-02-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(5-phenylpentyl)amino]propoxy]phenyl]-2-oxo-N-propyl-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

RN 782469-04-9 CAPLUS

CN Piperidine, 1-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(5-phenylpentyl)amino]propoxy]phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Ph
$$(CH_2)$$
 5 (CH_2) 3 (CH_2) 6 (CH_2) 8 (CH_2) 6 (CH_2) 8 (CH_2) 8 (CH_2) 9 (CH_2)

RN 782469-06-1 CAPLUS

CN 4-Piperidinol, 1-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(5-phenylpentyl)amino]propoxy]phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, rel- (9CI) (CA INDEX NAME)

Ph
$$(CH_2)_5$$
 $(CH_2)_3$ $(CH_2)_3$ $(CH_2)_4$ $(CH_2)_5$ (CH_2)

RN 782469-52-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-[3-[3-[3-(2-chlorophenyl)propyl]amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Me₃C
$$C_1$$
 C_1 C_1

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IT
     737784-68-8P 737784-69-9P 737784-70-2P
     782467-44-1P 782468-13-7P 782468-15-9P
     782468-17-1P 782468-25-1P 782468-27-3P
     782468-29-5P 782468-31-9P 782468-33-1P
     782468-35-3P 782468-39-7P 782468-41-1P
     782468-43-3P 782468-50-2P 782468-54-6P
     782468-56-8P 782468-58-0P 782468-60-4P
     782468-88-6P 782468-90-0P 782468-92-2P
     782469-51-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of benzoxazepine compds. as agents for controlling function of
        RFRP receptor)
RN
     737784-68-8 CAPLUS
```

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, ethyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 737784-69-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 737784-70-2 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

RN 782467-44-1 CAPLUS

CN 4,1-Benzoxazepine-1,3(5H)-diacetic acid, 7-chloro-2,3-dihydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, α1-(1,1-dimethylethyl) α3-methyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782468-13-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[methyl(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

RN 782468-15-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[[(2-nitrophenyl)sulfonyl](2-phenoxyethyl)amino]propoxy]phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782468-17-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(2-phenoxyethyl)amino]propoxy]phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

RN 782468-25-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, ethyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782468-27-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Meo
$$C1$$

Meo $C1$
 $C1$
 $C1$
 $CH_2)_3$
 $CH_2)_3$
 $CH_2)_3$

RN 782468-29-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-N-(phenylmethyl)-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

$$\begin{array}{c} \text{Me 3C} \\ \text{Ph} \\ \text{N} \\ \text{H} \end{array}$$

RN 782468-31-9 CAPLUS

CN Glycine, N-[[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, rel- (9CI) (CA INDEX NAME)

RN 782468-33-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, (3R,5S)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782468-35-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-1-methyl-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

RN 782468-39-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1-[(2,4-dimethoxyphenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, methyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782468-41-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1,2,3,5-tetrahydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

RN 782468-43-3 CAPLUS

CN 4,1-Benzoxazepine-1,3(5H)-diacetic acid, 7-chloro-2,3-dihydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, α 1-(1,1-dimethylethyl) α 3-methyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782468-50-2 CAPLUS

CN 4,1-Benzoxazepine-1,3(5H)-diacetic acid, 7-chloro-2,3-dihydro-5-[2-methoxy3-[3-[(2-nitrophenyl)sulfonyl](3-phenylpropyl)amino]propoxy]phenyl]-2-oxo, α1-(1,1-dimethylethyl) α3-methyl ester, (3R,5S)-rel- (9CI)
(CA INDEX NAME)

RN 782468-54-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-[3-[3-[3-(2-chlorophenyl)propyl]methylamino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782468-56-8 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-[3-[(3-phenylpropyl)amino]propoxy]phenyl]-2-oxo-, 4-piperidinyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Ph
$$(CH_2)_3$$
 $(CH_2)_3$ (CH_2)

RN 782468-58-0 CAPLUS

CN 2-Piperazinecarboxylic acid, 4-[[(3R,5S)-7-chloro-5-[3-[3-[[(1,1-dimethylethoxy)carbonyl](3-phenylpropyl)amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782468-60-4 CAPLUS

CN 1,2-Piperazinedicarboxylic acid, 4-[[(3R,5S)-7-chloro-5-[3-[3-[[(1,1-dimethylethoxy)carbonyl](3-phenylpropyl)amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, 1-(1,1-dimethylethyl) 2-ethyl ester, rel- (9CI) (CA INDEX NAME)

RN 782468-88-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1-[(2,4-dimethoxyphenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, ethyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782468-90-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1-[(2,4-dimethoxyphenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

RN 782468-92-2 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-[(2,4-dimethoxyphenyl)methyl]-N[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3(phenylmethoxy)phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 782469-51-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-[3-[3-[3-[3-(2-chlorophenyl)propyl]amino]propoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester, (3R,5s)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Meo Cl
$$(CH_2)_3$$
 $(CH_2)_3$ $(CH_2)_3$ $(CH_2)_3$

REFERENCE COUNT:

THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/256,198

ANSWER 5 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACKESSION NUMBER: 2004:648392 CAPLUS

DOCUMENT NUMBER: 141:190808

TITLE: Preparation of aromatic ring-fused cyclic compounds as

TGR5 receptor agonists

INVENTOR(S): Itoh, Fumio; Hinuma, Shuji; Kanzaki, Naoyuki; Miki,

Takashi; Kawamata, Yuji; Oi, Satoru; Tawaraishi,

Taisuke; Ishichi, Yuji; Hirohashi, Mariko Takeda Chemical Industries, Ltd., Japan

PATENT ASSIGNEE(S): Takeda Chemical Industr SOURCE: PCT Int. Appl., 337 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Patent
Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.				KIND DATE					APPLICATION NO.					DATE			
					- \												
WO 2004067008				A1 20040812				,	WO 2004-JP706					20040127			
W:	ΑE,	ΑE,	ΑG,	AL,	AL,	AM,	_MA_	AM,	AT,	AT,	ΑU,	ΑZ,	ΑZ,	BA,	BB,	BG,	
	BG,	BR,	BR,	BW,	BY,	BY,	BZ,	BZ,	CA,	CH,	CN,	CN,	co,	CO,	CR,	CR,	
	CU,	CU,	CZ,	CZ,	DE,	DE,	DK,	DK,	DM,	DZ,	EC,	EC,	EE,	EE,	EG,	ES,	
	ES,	FI,	FI,	GB,	GD,	GE,	GE,	GH,	GM,	HR,	HR,	HU,	HU,	ID,	IL,	IN,	
	IS,	JP,	JP,	KE,	KE,	KG,	KG,	KP,	KP,	KP,	KR,	KR,	ΚZ,	ΚZ,	ΚZ,	LC,	
	LK,	LR,	LS,	LS,	LT,	LU,	LV,	MA,	MD,	MD,	MG,	MK,	MN,	MW,	MX,	MX,	
	MZ,	MZ,	NA,	NI													
JP 2004346059				A2	20041209 JP 2004-18643							20040127					
PRIORITY APPLN. INFO.:								JP 2003-19272				A 20030128					
									JP 2	003-	1243	11	1	A 2	0030	428	

OTHER SOURCE(S): MARPAT 141:190808

GΙ



AB It is intended to provide G protein-coupled receptor (TGR5) agonists containing fused ring compds. represented by the following general formula (I), salts or prodrugs thereof (wherein the ring A represents an optionally substituted aromatic ring; and the ring B represents a 5- to 8-membered ring having one or more substituents). Also disclosed are regulators for physiol. functions involving TGR5, preventives and/or remedies for various diseases involving TGR5, cytokine production inhibitors, GLP-1 secretion promoters, insulin secretion promoters, appetite depressants, pancreas regenerants, promoters for pancreas β -cell differentiation or proliferation, insulin resistance improvers, or immunosuppressants. containing the compds. I. In particular disclosed are preventives and/or remedies containing the compds. I for heart failure, myocardial infarction, acute kidney failure, angina pectoris, arrhythmia, bronchial asthma, chronic obstructive pulmonary disease, arteriosclerosis, chronic articular rheumatism, diabetes, obesity, insulin secretion failure, pancreas fatigue, gastric ulcer, ulcerative colitis, allergy, osteoarthritis, erythematodes, or excessive immune reaction after transplant surgery. The compds. I are also useful for screening ligands,

agonists, or antagonists of TGR5. Thus, 0.1 g 2-[trans-7-chloro-5-(3-formylphenyl)-1-neopentyl-2-oxo-1,2,3,5-tetrahydro-4,1-benzoxazepin-3-yl]-N-(2-fluorobenzyl)acetamide was reduced by NaBH4 in MeOH at room temperature

for

30 min to give 76 mg 2-[trans-7-chloro-5-(3-hydroxyphenyl)-1-neopentyl-2-oxo-1,2,3,5-tetrahydro-4,1-benzoxazepin-3-yl]-N-(2-fluorobenzyl)acetamide (II). II at 1 μ M increased the production of cAMP in CHO cells expressing human TGR5 by 128%. Pharmaceutical formulations containing specific compound I were also prepared

IT 737785-03-4P 737785-06-7P 737785-08-9P 737785-09-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aromatic ring-fused cyclic compds. as ${\tt TGR5}$ receptor agonists,

cytokine production inhibitors and appetite depressants)

RN 737785-03-4 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 5-[3-(2-amino-2-oxoethoxy)-2-methoxyphenyl]-7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 737785-06-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-[3-[2-(dimethylamino)-2-oxoethoxy]-2-methoxyphenyl]-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)-rel- (9CI) (CFINDEX NAME)

RN 737785-08-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-[2-oxo-2-[(2-phenylethyl)amino]ethoxy]phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 737785-09-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[3-[2-[[3-(1H-imidazol-1-yl)propyl]amino]-2-oxoethoxy]-2-methoxyphenyl]-2-oxo-, (3R,5S)-rel-(9CI) (CA INDEX NAME)

IT 737784-68-8P 737784-69-9P 737784-70-2P 737784-72-4P 737784-73-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aromatic ring-fused cyclic compds. as TGR5 receptor agonists,

cytokine production inhibitors and appetite depressants)

RN 737784-68-8 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, ethyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 737784-69-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, (3R,5S)-rel-(9CI) (CA INDEX NAME)

RN 737784-70-2 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-1-(2,2-dimethylpropyl)-N-[(2-fluorophenyl)methyl]-1,2,3,5-tetrahydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 737784-72-4 CAPLUS

CN Acetic acid, [3-[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-3-[2-[[(2-fluorophenyl)methyl]amino]-2-oxoethyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-5-yl]-2-methoxyphenoxy]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

RN

737784-73-5 CAPLUS
Acetic acid, [3-[(3R,5S)-7-chloro-1-(2,2-dimethylpropyl)-3-[2-[[(2-fluorophenyl)methyl]amino]-2-oxoethyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-5-yl]-2-methoxyphenoxy]-, rel- (9CI) (CA INDEX NAME) CN

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ANSWER 6 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
ASCESSION NUMBER:
                                               2004:633548 CAPLUS
DOCUMENT NUMBER:
                                               141:162403
                                               Skeletal muscle protecting agents containing squalene
TITLE:
                                               synthase inhibitors
                                               Tozawa, Ryuichi; Nishimoto, Tomoyuki
INVENTOR(S):
                                               Takeda Chemical Industries, Ltd., Japan
PATENT ASSIGNEE(S):
                                               PCT Int. Appl., 94 pp.
SOURCE:
                                               CODEN: PIXXD2
DOCUMENT TYPE:
                                               Patent
LANGUAGE:
                                                Japanese
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
         PATENT NO.
                                                             DATE
                                                                                                                             DATE
                                               KIND
                                                                                  APPLICATION NO.
                                                              /----
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                                                            (20040805
                                                                                   )WO 2004-JP234
                                                                                                                             20040115
         WO 2004064865
                                                 A1
                 W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AU, AZ, AZ, BA, BB,
                        BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR,
                        CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG,
                        ES, ES, FI, FI, GB, GD, GE, GE, GH, GH, GH, GM, HR, HR, HU, HU,
                         ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ,
                        KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN,
                        MW, MX, MX, MZ
          JP 2003277377
                                                 A2
                                                             20031002
                                                                                    JP 2003-10125
                                                                                                                                20030117
PRIORITY APPLN. INFO.:
                                                                                    JP 2003-10125
                                                                                                                       A 20030117
                                                                                    JP 2003-93591
                                                                                                                        A 20030331
                                                                                    JP 2002-10623
                                                                                                                        A 20020118
OTHER SOURCE(S):
                                               MARPAT 141:162403
          It is intended to provide a novel drug useful as a skeletal muscle
          protecting agent which contains a compound having an effect of inhibiting
          squalene synthase, its salt or a prodrug thereof. The agent of the
          present invention is suitable for use for protecting skeletal muscle from
          cytotoxicity due to usage of other drug, e.g. HMG-CoA reductase inhibitor.
          The effect of N-[(3R,5S)-1-(3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-5-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-6-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-6-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-6-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-6-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-6-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-6-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-6-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-6-(2,3-acetoxy-2,2-dimethylpropy1)-7-chloro-6-(2,3-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetoxy-2,2-acetox
          dimethoxyphenyl)-2-oxo-1,2,3,5-tetrahydro-4,1-benzoxazepin-3-
          yl]acetyl]piperidine-4-acetic acid on muscle geranylgeraniol content in
          rats was examined
IT
          189059-71-0 189060-13-7 383652-98-0
          RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
          (Biological study); USES (Uses)
                (skeletal muscle protecting agents containing squalene synthase inhibitors)
          189059-71-0 CAPLUS
          4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-
CN
          1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-
          3-yl]acetyl]- (9CI) (CA INDEX NAME)
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RN 189060-13-7 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383652-98-0 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

REFERENCE COUNT:

THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/256, 198

ANSWER 7 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:885310 CAPLUS

DOCUMENT NUMBER: 140:174823

TITLE: Comparing myotoxic effects of squalene synthase

inhibitor, T-91485, and 3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase inhibitors in human

myocytes

Nishimoto, Tomoyuki; Tozawa, Ryuichi; Amano, Yuichiro; AUTHOR(S):

Wada, Takeo; Imura, Yoshimi; Sugiyama, Yasuo

Pharmaceutical Research Division, Pharmacology CORPORATE SOURCE:

Research Laboratories I, Takeda Chemical Industries, Ltd., Yodogawa-ku, Osaka, 532-8686, Japan Biochemical Pharmacology (2003), 66(11), 2133-2139

SOURCE:

CODEN: BCPCA6; ISSN: 006-2952

Elsevier Science B.V. PUBLISHER:

Journal DOCUMENT TYPE: English LANGUAGE:

TAK-475 is a squalene synthase inhibitor, rapidly metabolized to T-91485 in vivo. We investigated the myotoxicities of T-91485 and 3-hydroxy-3-methylglutaryl CoA (HMG-CoA) reductase inhibitors in a human rhabdomyosarcoma cell line, RD, and in human skeletal myocytes. In differentiated RD cells, T-91485, atorvastatin (ATV) and simvastatin acid (SIM) inhibited cholesterol biosynthesis, with ic50 values of 36, 2.8 and 3.8 nM, resp. ATV and SIM decreased the intracellular ATP content, with ic25 values (concns. giving a 25% decrease in intracellular ATP content) of 0.61 and 0.44 µM, resp. Although T-91485 potently inhibited cholesterol synthesis in RD cells, the ic25 value exceeded 100 μM . human skeletal myocytes, T-91485, ATV and SIM concentration-dependently

cholesterol biosynthesis, with ic50 values of 45, 8.6 and 8.4 nM, resp. ATV and SIM decreased intracellular ATP content, with ic25 values of 2.1 and 0.72 µM, resp. Although T-91485 potently inhibited cholesterol synthesis, the ic25 value exceeded 100 µM. Myotoxicity induced by ATV was prevented by mevalonate or geranylgeranyl-PP, but not by squalene in skeletal cells. Furthermore, T-91485 attenuated the myotoxicity of ATV. These findings suggest that TAK-475 and T-91485 may not only be far from myotoxic, they may also decrease statin-induced myotoxicity in lipid-lowering therapy.

189059-71-0, T 91485 IT

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (comparing myotoxic effects of squalene synthase inhibitor, T-91485, and 3-hydroxy-3-methylglutaryl CoA (HMG-CoA) reductase inhibitors in human myocytes)

RN 189059-71-0 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/256,198

INVENTOR(S):

ANSWER 8 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:767796 CAPLUS

DOCUMENT NUMBER: 139:276921

TITLE: Preparation of benzoxazepine derivatives as squalene

synthetic enzyme inhibitors Miki, Takashi; Kori, Masaki

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 36 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

	1117		
	1117		
JP 2003277377 A2 20031002 JP 2003-10125 2003	20030117		
WO 2004064865 A1 20040805 WO 2004-JP234 2004	20040115		
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AU, AZ, AZ, BA	BB,		
BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO	. CR,		
CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE	EG,		
ES, ES, FI, FI, GB, GD, GE, GE, GH, GH, GH, GM, HR, HR, HU	HU,		
ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR	KZ,		
KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK	, MN,		
MW, MX, MX, MZ			
JP 2004107361 A2 20040408 JP 2004-9836 2004)116		
JP 2004315500 A2 20041111 JP 2004-9617 2004)116		
PRIORITY APPLN. INFO.: JP 2002-10623 A 2002)118		
JP 2003-10125 A 2003)117		
JP 2003-93591 A 2003)331		

OTHER SOURCE(S): MARPAT 139:276921

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [wherein W = halo; R1 = alkyl; R2 = CHO or (un)substituted alkyl; m = 1-3; n = 0-2; R4 = H or -(CH2)p-R5; R5 = (un)substituted CO2H; p = 0-3; etc.] and salts and prodrugs thereof are prepared as squalene synthetic enzyme inhibitors. I are useful as a lipid decrease medicine and a high fat blood disease medicine (no data). Thus, the compound II was prepared in a multi-step synthesis. II showed IC50 of 45 nM against human squalene synthetic enzyme. Formulations containing I as an active ingredient were also described.

IT 606928-79-4P

RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(drug candidate; preparation of benzoxazepine derivs. as squalene synthetic enzyme inhibitors)

RN 606928-79-4 CAPLUS

CN 4-Pyridineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,4-tetrahydro-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 606928-80-7P 606928-81-8P

RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzoxazepine derivs. as squalene synthetic enzyme inhibitors)

RN 606928-80-7 CAPLUS

CN 4-Pyridineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,4-tetrahydro-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 606928-81-8 CAPLUS

CN 4-Pyridineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,4-tetrahydro-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 606928-73-8P 606928-75-0P 606928-77-2P 606928-78-3P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; preparation of benzoxazepine derivs. as squalene synthetic enzyme inhibitors)

RN 606928-73-8 CAPLUS

CN 4-Pyridineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,6-tetrahydro-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 606928-75-0 CAPLUS

CN Pyridine, 1-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,4-tetrahydro-(9CI) (CA INDEX NAME)

RN 606928-77-2 CAPLUS

CN 4-Pyridineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethyl-3-oxopropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,4-tetrahydro-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 606928-78-3 CAPLUS

CN 4-Pyridineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,4-tetrahydro-, methyl ester (9CI) (CA INDEX NAME)

IT 383652-98-0P 606928-74-9P 606928-76-1P 606929-11-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzoxazepine derivs. as squalene synthetic enzyme inhibitors)

RN 383652-98-0 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 606928-74-9 CAPLUS

CN 4-Pyridineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,6-tetrahydro-(9CI) (CA INDEX NAME)

RN 606928-76-1 CAPLUS

CN Pyridine, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,4-tetrahydro-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 606929-11-7 CAPLUS

CN 4-Pyridineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-1,2,3,4-tetrahydro-(9CI) (CA INDEX NAME)

IT 606928-85-2P 606928-96-5P 606928-97-6P 606928-98-7P 606929-00-4P 606929-01-5P 606929-02-6P 606929-03-7P 606929-04-8P 606929-06-0P 606929-07-1P 606929-08-2P 606929-09-3P 606929-10-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; preparation of benzoxazepine derivs. as squalene synthetic enzyme inhibitors) RN 606928-85-2 CAPLUS CN 4,1-Benzoxazepine-3-acetamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-N-(5-hydroxypentyl)-2oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 606928-96-5 CAPLUS
CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-N-[2-(tetrahydro-2-oxo-2H-pyran-4-yl)ethyl]-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 606928-97-6 CAPLUS

CN Pentanoic acid, 3-[2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]-5-hydroxy-, monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Na

RN 606928-98-7 CAPLUS

CN Pentanoic acid, 3-[2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]-5-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

RN 606929-00-4 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, ethyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 606929-01-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

RN 606929-02-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-1,2,3,5-tetrahydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 606929-03-7 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-1,2,3,5-tetrahydro-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester, rel- (9CI) (CA INDEX NAME)

RN 606929-04-8 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-5-[2-methoxy-3-(phenylmethoxy)phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 606929-06-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-5-[3-methoxy-2-(phenylmethoxy)phenyl]-2-oxo-, ethyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

RN 606929-07-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-5-[3-methoxy-2-(phenylmethoxy)phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 606929-08-2 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-1,2,3,5-tetrahydro-5-[3-methoxy-2-(phenylmethoxy)phenyl]-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

RN 606929-09-3 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-1,2,3,5-tetrahydro-5-[3-methoxy-2-(phenylmethoxy)phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 606929-10-6 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-5-[3-methoxy-2-(phenylmethoxy)phenyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, rel- (9CI) (CA INDEX NAME)

IT 189060-51-3 383661-55-0

RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of benzoxazepine derivs. as squalene synthetic enzyme
 inhibitors)

RN 189060-51-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383661-55-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

10/256,198

ANSWER 9 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:584090 CAPLUS

DOCUMENT NUMBER: 139:240092

TTILE: Lipid-lowering properties of TAK-475, a squalene

synthase inhibitor, in vivo and in vitro

AUTHOR(S): Nishimoto, Tomoyuki; Amano, Yuichiro; Tozawa, Ryuichi;

Ishikawa, Eiichiro; Imura, Yoshimi; Yukimasa,

Hidefumi; Sugiyama, Yasuo

CORPORATE SOURCE: Pharmacology Research Laboratories I, Pharmaceutical

Research Division, Takeda Chemical Industries, Ltd,

Osaka, 532-8686, Japan

SOURCE: British Journal of Pharmacology (2003), 139(5),

911-918

CODEN: BJPCBM; ISSN: 0007-1188

PUBLISHER: Nature Publishing Group

DOCUMENT TYPE: Journal LANGUAGE: English

Squalene synthase is the enzyme that converts farnesyl pyrophosphate to squalene in the cholesterol biosynthesis pathway. We examined the lipid-lowering properties of 1-[[(3R,5S)-1-(3- acetoxy-2,2-dimethylpropyl)-7-chloro-5-(2,3-dimethoxyphenyl)- 2-oxo-1,2,3,5-tetrahydro- 4,1-benzoxazepin-3-yl]acetyl]piperidine- 4-acetic acid (TAK-475), a novel squalene synthase inhibitor. TAK-475 inhibited hepatic cholesterol biosynthesis in rats (ED50, 2.9 mg kg-1) and showed lipid-lowering effects in beagle dogs, marmosets, cynomolgus monkeys and Wistar fatty rats. In marmosets, TAK-475 (30, 100 mg kg-1, p.o., for 4 days) lowered both plasma non-high-d. lipoprotein (HDL) cholesterol and triglyceride, but did not affect plasma HDL cholesterol. Atorvastatin (10, 30 mg kg-1, p.o., for 4 days) lowered the levels of all these lipids. A correlation between decrease in triglyceride and increase in HDL cholesterol was observed, and TAK-475 increased HDL cholesterol with a smaller decrease in triglyceride than did atorvastatin. TAK-475 (60 mg kg-1, p.o., for 15 days) suppressed the rate of triglyceride secretion from the liver in hypertriglyceridemic Wistar fatty rats, which show an enhanced triglyceride secretion rate from the liver compared with their lean littermates. In HepG2 cells, TAK-475 and its pharmacol. active metabolite, T-91485, increased the binding of 125I-low-d. lipoprotein (LDL) to LDL receptors. These results suggest that TAK-475 has clear hypolipidemic effects in animals via inhibition of hepatic triglyceride secretion and upregulation of LDL receptors, and that TAK-475 might increase HDL cholesterol by decreasing triglyceride. Thus, TAK-475 is expected to be useful for the treatment of dyslipidemia.

IT 189060-13-7, TAK 475

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (lipid-lowering properties of TAK-475)

RN 189060-13-7 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

IT 189059-71-0

RL: PAC (Pharmacological activity); BIOL (Biological study) (lipid-lowering properties of TAK-475)

RN 189059-71-0 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/25/6.198 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2003:249806 CAPLUS DOCUMENT NUMBER: 139:173582 Lipid-lowering effects of TAK-475, a squalene synthase TITLE: inhibitor, in animal models of familial hypercholesterolemia Amano, Yuichiro; Nishimoto, Tomoyuki; Tozawa, AUTHOR(S): Ryu-Ichi; Ishikawa, Eiichiro; Imura, Yoshimi; Suqiyama, Yasuo CORPORATE SOURCE: Pharmaceutical Research Division, Pharmacology Research Laboratories II, Takeda Chemical Industries, Ltd., 2-17-85, Juso-Honmachi, Osaka, Yodogawa, 532-8686, Japan European Journal of Pharmacology (2003), 466(1-2), SOURCE: 155-161 CODEN: EJPHAZ; ISSN: 0014-2999 PUBLISHER: Elsevier Science B.V. Journal DOCUMENT TYPE: English LANGUAGE: The lipid-lowering effects of $1-\{2-\{(3R,5S)-1-(3-acetoxy-2,2-ace$ dimethylpropyl)-7-chloro-1,2,3,5-tetrahydro-2-oxo-5-(2,3-dimethoxyphenyl)-4,1-benzoxazepine-3-yl] acetyl} piperidin-4-acetic acid (TAK-475), a novel squalene synthase inhibitor, were examined in two models of familial hypercholesterolemia, low-d. lipoprotein (LDL) receptor knockout mice and Watanabe heritable hyperlipidemic (WHHL) rabbits. Two weeks of treatment with TAK-475 in a diet admixt. (0.02% and 0.07%; approx. 30 and 110 mg/kg/day, resp.) significantly lowered plasma non-high-d. lipoprotein (HDL) cholesterol levels by 19% and 41%, resp., in homozygous LDL receptor knockout mice. The 3-hydroxy-3-methylglutaryl CoA (HMG-CoA) reductase inhibitors, simvastatin and atorvastatin (in 0.02% and 0.07% admixts.), also reduced plasma levels of non-HDL cholesterol. In homozygous WHHL rabbits, 4 wk of treatment with TAK-475 (0.27%; approx. 100 mg/kg/day) lowered plasma total cholesterol, triglyceride and phospholipid levels by 17%, 52% and 26%, resp. In Triton WR-1339-treated rabbits, TAK-475 inhibited to the same extent the rate of secretion from the liver of the cholesterol, triglyceride and phospholipid components of very-low-d. lipoprotein (VLDL). These results suggest that the lipid-lowering effects of TAK-475 in WHHL rabbits are based partially on the inhibition of secretion of VLDL from the liver. TAK-475 had no effect on plasma aspartate aminotransferase and alanine aminotransferase activities. the squalene synthase inhibitor TAK-475 revealed lipid-lowering effects in both LDL receptor knockout mice and WHHL rabbits. 189060-13-7, TAK 475 ITRL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (lipid-lowering effects of TAK-475, a squalene synthase inhibitor, in animal models of familial hypercholesterolemia) 189060-13-7 CAPLUS RN

4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-

7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-

Absolute stereochemistry.

3-yl]acetyl]- (9CI) (CA INDEX NAME)

CN

REFERENCE COUNT:

32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:22711 CAPLUS

DOCUMENT NUMBER: 138:83384

TITLE: Preventives/remedies for organ functional disorders

with increasing ubiquinone and inhibiting squalene

synthase

INVENTOR(S): Sugiyama, Yasuo; Nishimoto, Tomoyuki; Kiyota,

Yoshihiro

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 121 pp.

CODEN: PIXXD2

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DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	PATENT NO.					KIND DATE			APPLICATION NO.							DATE			
W	0 2003002147				A1 20030109			WO 2002-JP6495						20020627					
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,		
		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,		
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KR,	ΚZ,	LC,	LK,	LR,	LS,		
		LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	ΝZ,	OM,	PH,	PL,		
		PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,		
		ŪG,	US,	UZ,	VN,	YU,	ZA,	ZM,	ZW,	AM,	AZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM	
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AT,	BE,	CH,		
		CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,		
		BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG		
CZ	CA 2451163				AA	AA 20030109				CA 2002-2451163					20020627				
JI	JP 2003081873				A2	2 20030319			JP 2002-188133					20020627					
El	EP 1407782				A1 20040414			EP 2002-738822					20020627						
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,		
		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR								
បះ	US 2004204500				A1		20041014			US 2003-480707					20031211				
PRIORI	PRIORITY APPLN. INFO.:									JP 2001-197419				1	A 2	0010	628		
									1	WO 2	002-	JP64:	95	Ţ	W 2	0020	627		

OTHER SOURCE(S): MARPAT 138:83384

AB Preventives/remedies for organ functional disorders, preventives/remedies for organ dysfunction and preventives/remedies for obesity and sequels thereof which contain a compound having an effect of increasing ubiquinone, its salt or prodrugs of the same; and ubiquinone increasing agents containing a compound having a squalene synthase inhibitory effect, its salt or prodrugs of the same.

IT 383652-98-0P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Preventives/remedies for organ functional disorders with increasing ubiquinone and inhibiting squalene synthase)

RN 383652-98-0 CAPLUS

CN Benzenepropanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

```
IT
     171868-39-6 189058-78-4, N-[[(3R,5S)-1-(2,2-
     Dimethylpropyl)-7-chloro-5-(2,3-dimethoxyphenyl)-2-oxo-1,2,3,5-tetrahydro-
     4,1-Benzoxazepin-3-yl]acetyl]piperidineacetic acid 189059-19-6
     189059-57-2 189059-71-0, N-[[(3R,5S)-1-(3-Hydroxy-2,2-
     dimethylpropyl)-7-chloro-5-(2,3-dimethoxyphenyl)-2-oxo-1,2,3,5-tetrahydro-
     4,1-Benzoxazepin-3-yl]acetyl]piperidineacetic acid 189059-84-5
     189059-85-6 189060-04-6, Ethyl N-[[(3R,5S)-1-(3-Acetoxy-
     2-acetoxy-2-methylpropyl)-7-chloro-5-(2,3-dimethoxyphenyl)-2-oxo-1,2,3,5-
     tetrahydro-4,1-Benzoxazepin-3-yl]acetyl]piperidineacetate
     189060-07-9 189060-10-4, Ethyl N-[[(3R,5S)-1-(3-Acetoxy-
     2,2-dimethylpropyl)-7-chloro-5-(2,3-dimethoxyphenyl)-2-oxo-1,2,3,5-
     tetrahydro-4,1-benzoxazepin-3-yl]acetyl]piperidineacetate
     189060-21-7 189060-33-1 189060-37-5
     189060-41-1 189060-45-5 189060-48-8
     383652-05-9 383652-11-7 383652-16-2
     383652-22-0 383652-28-6 383652-33-3
     383652-38-8 383652-44-6, Benzenepropanoic acid,
     3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-
     hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-
     methyl- 383652-50-4 383652-56-0 383652-61-7
     383652-66-2 383652-71-9 383652-76-4
     383652-81-1 383652-87-7 383652-92-4
     383654-65-7, Benzenepropanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-
     dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-
     4,1-benzoxazepin-3-yl]acetyl]amino]- 383657-83-8
     383662-50-8
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (Preventives/remedies for organ functional disorders with increasing
        ubiquinone and inhibiting squalene synthase)
RM
     171868-39-6 CAPLUS
CN
     4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-
     dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)
```

RN 189058-78-4 CAPLUS

CN 4-Piperidineacetic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-19-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-N-[2-(1-pyrrolidinyl)ethyl]-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189059-57-2 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-1-(3-hydroxy-2,2-dimethylpropyl)-3-(1H-tetrazol-5-ylmethyl)-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-71-0 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 189059-84-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-N-(methylsulfonyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-85-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[3-hydroxy-2-(hydroxymethyl)-2-methylpropyl]-N-(methylsulfonyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189060-04-6 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2-[(acetyloxy)methyl]-2-methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-07-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 1-[3-(acetyloxy)-2-[(acetyloxy)methyl]-2-methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-N-(methylsulfonyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189060-10-4 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-21-7 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-1-[3-hydroxy-2-(hydroxymethyl)-2-methylpropyl]-3-(1H-tetrazol-5-ylmethyl)-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189060-33-1 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2-[(acetyloxy)methyl]-2-methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-3-(1H-tetrazol-5-ylmethyl)-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-37-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[3-hydroxy-2-(hydroxymethyl)-2-methylpropyl]-2-oxo-N-[2-(1-pyrrolidinyl)ethyl]-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189060-41-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-N-[2-(1-pyrrolidinyl)ethyl]-1-[(2,2,5-trimethyl-1,3-dioxan-5-yl)methyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-45-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-N-(methylsulfonyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189060-48-8 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-3-(1H-tetrazol-5-ylmethyl)-, (3R,5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383652-05-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-N-(propylsulfonyl)-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 383652-11-7 CAPLUS

CN D-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-16-2 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383652-22-0 CAPLUS

CN Butanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-28-6 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, trans- (9CI) (CA INDEX NAME)

RN 383652-33-3 CAPLUS

Cyclohexanecarboxylic acid, 4-[[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, trans- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-38-8 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro- (9CI) (CA INDEX NAME)

RN 383652-44-6 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383652-50-4 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

RN 383652-56-0 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383652-61-7 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 383652-66-2 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-71-9 CAPLUS

CN Benzenebutanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy- (9CI) (CA INDEX NAME)

RN 383652-76-4 CAPLUS

CN Benzenepentanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-81-1 CAPLUS

CN Benzenepentanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro-(9CI) (CA INDEX NAME)

RN 383652-87-7 CAPLUS

CN 3-Furancarboxylic acid, 2-[2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-92-4 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro-(9CI) (CA INDEX NAME)

RN 383654-65-7 CAPLUS

CN Benzenepropanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383657-83-8 CAPLUS

CN 2-Furancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383662-50-8 CAPLUS

CN 3-Furancarboxylic acid, 2-[2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 189060-51-3P, (3R,5S)-7-Chloro-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-5-(2,3-dimethoxyphenyl)-2-oxo-4,1-benzoxazepin-3-acetic acid 383654-76-0P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(Preventives/remedies for organ functional disorders with increasing ubiquinone and inhibiting squalene synthase)

RN 189060-51-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383654-76-0 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 189060-13-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(Preventives/remedies for organ functional disorders with increasing ubiquinone and inhibiting squalene synthase)

RN 189060-13-7 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/256,198

ANSWER 12 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:664428 CAPLUS

DØCMMENT NUMBER: 137:337866

TITLE: Synthesis of Novel 4,1-Benzoxazepine Derivatives as

Squalene Synthase Inhibitors and Their Inhibition of

Cholesterol Synthesis

AUTHOR(S): Miki, Takashi; Kori, Masakuni; Mabuchi, Hiroshi;

Tozawa, Ryu-ichi; Nishimoto, Tomoyuki; Sugiyama,

Yasuo; Teshima, Koichiro; Yukimasa, Hidefumi

CORPORATE SOURCE: Pharmaceutical Research Division, Takeda Chemical

Industries Ltd., Yodogawa-ku, Osaka, \$32-8686, Japan

Journal of Medicinal Chemistry (2002) 45(20),

4571-4580

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

SOURCE:

Journal English

LANGUAGE:
OTHER SOURCE(S):

CASREACT 137:337866

GT

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Modification of the carboxyl group at the 3-position and introduction of protective groups to the hydroxy group of the 4,1-benzoxazepine derivative I (R = OH) [metabolite of I (R = H) Na salt] were carried out, and the inhibitory activity for squalene synthase and cholesterol synthesis in the liver was investigated. Among these compds., the glycine derivative II (n = 1) and β -alanine derivative II (n = 2) exhibited the most potent inhibition of squalene synthase prepared from HepG2 cells (IC50 = 15 nM). On the other hand, the piperidine-4-acetic acid derivative III (R1 = Ac), which was prepared by acetylation of III (R1 = H), was the most effective inhibitor of cholesterol synthesis in rat liver (ED50 = 2.9 mg/kg, po). After oral administration, III (R1 = Ac) was absorbed and rapidly hydrolyzed to III (R1 = H). Compound III (R1 = H) was detected mainly in the liver, but the plasma level of III (R1 = H) was found to be low. Compds. III (R1 = H, Ac) were found to be competitive inhibitors with respect to farnesyl pyrophosphate. Further evaluation of III (Rl = Ac) as a cholesterol-lowering and antiatherosclerotic agent is underway.

IT 189059-71-0P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 4,1-benzoxazepines as squalene synthase inhibitors and their inhibition of cholesterol synthesis)

RN 189059-71-0 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

IT 189059-72-1P 189060-13-7P 383653-71-2P 383654-03-3P 383654-14-6P 383658-74-0P 383658-84-2P 473987-15-4P 473987-16-5P 473987-17-6P 473987-18-7P 473987-19-8P 473987-25-6P 473987-26-7P 473987-27-8P 473987-28-9P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation of 4,1-benzoxazepines as squalene synthase inhibitors and their inhibition of cholesterol synthesis) RN 189059-72-1 CAPLUS CN 4-Piperidinecarboxylic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-13-7 CAPLUS
CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383653-71-2 CAPLUS

CN D-Leucine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383654-03-3 CAPLUS

CN L-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

RN 383654-14-6 CAPLUS

CN D-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383658-74-0 CAPLUS

CN Butanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383658-84-2 CAPLUS

CN Pentanoic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 473987-15-4 CAPLUS

CN Glycine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 473987-16-5 CAPLUS

CN Glycine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 473987-17-6 CAPLUS

CN β-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 473987-18-7 CAPLUS

CN 4-Piperidinepropanoic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 473987-19-8 CAPLUS

CN 4-Piperidinebutanoic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 473987-25-6 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[2,2-dimethyl-3-(1-oxopropoxy)propyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 473987-26-7 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1[2,2-dimethyl-3-(1-oxobutoxy)propyl]-1,2,3,5-tetrahydro-2-oxo-4,1benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 473987-27-8 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1[2,2-dimethyl-3-(2-methyl-1-oxopropoxy)propyl]-1,2,3,5-tetrahydro-2-oxo4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 473987-28-9 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[3-[(2,2-dimethyl-1-oxopropoxy)methoxy]-2,2-dimethylpropyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

IT189059-61-8P 189059-65-2P 189059-66-3P 189060-51-3P 383661-79-8P 383662-10-0P 383662-15-5P 383669-08-7P 383669-14-5P 473987-08-5P 473987-09-6P 473987-10-9P 473987-13-2P 473987-14-3P 473987-20-1P 473987-21-2P 473987-22-3P 473987-23-4P 473987-24-5P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of 4,1-benzoxazepines as squalene synthase inhibitors and their inhibition of cholesterol synthesis) 189059-61-8 CAPLUS RN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-CN tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-, ethyl ester, (3R,5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-65-2 CAPLUS
CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-

1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-66-3 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-51-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 383661-79-8 CAPLUS

CN D-Leucine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383662-10-0 CAPLUS

CN L-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383662-15-5 CAPLUS

CN D-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383669-08-7 CAPLUS

CN Butanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 383669-14-5 CAPLUS

CN Pentanoic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 473987-08-5 CAPLUS

CN Glycine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 473987-09-6 CAPLUS

CN Glycine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-N-methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 473987-10-9 CAPLUS

CN β-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 473987-13-2 CAPLUS

CN 4-Piperidinepropanoic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 473987-14-3 CAPLUS

CN 4-Piperidinebutanoic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 473987-20-1 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 473987-21-2 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1[2,2-dimethyl-3-(1-oxopropoxy)propyl]-1,2,3,5-tetrahydro-2-oxo-4,1benzoxazepin-3-yl]acetyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 473987-22-3 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[2,2-dimethyl-3-(1-oxobutoxy)propyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 473987-23-4 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[2,2-dimethyl-3-(2-methyl-1-oxopropoxy)propyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 473987-24-5 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-[3-[(2,2-dimethyl-1-oxopropoxy)methoxy]-2,2-dimethylpropyl]-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

REFERENCE COUNT:

32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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10/256,198
    ANSWER 13 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:
                        2002:368342 CAPLUS
DOCUMENT NUMBER:
                        136:359669
TITLE:
                        High-density lipoprotein-cholesterol level elevating
                        Nishimoto, Tomoyuki; Tozawa, Ryuichi; Kori, Masakuni;
INVENTOR(S):
                        Amano, Yuichiro
PATENT ASSIGNEE(S):
                        Takeda Chemical Industries, Ltd., Japan
                        PCT Int. Appl., 111 pp.
SOURCE:
                        CODEN: PIXXD2
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                        Patent
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FAMILY ACC. NUM. COUNT:
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                                                                  20030506
PRIORITY APPLN. INFO.:
                                           JP 2000-342607
                                                              A 20001109
                                                              W 20011109
                                           WO 2001-JP9802
                        MARPAT 136:359669
OTHER SOURCE(S):
     Disclosed is a novel high-d. lipoprotein (HDL)-cholesterol level elevating
AB
     agent containing a compound which has a squalene synthase inhibitory effect.
     The HDL-cholesterol-elevating effect of N-[[(3R,5S)-1-(3-acetoxy-2,2-
     dimethylpropyl)-7-chloro-5-(2,3-dimethoxyphenyl)-2-oxo-1,2,3,5-tetrahydro-
     4,1-benzoxazepine-3-yl]acetyl]piperidine-4-acetic acid (I) in common
     marmoset was examined Also, a tablet containing I 50, D-mannitol 50, corn
     starch 33.9, croscarmellose sodium 40, hydroxypropyl cellulose 5.5, and
     magnesium stearate 0.6 mg was prepared
IT
     189060-05-7
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (high-d. lipoprotein-cholesterol level elevating agents containing squalene
        synthase inhibitors)
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189060-05-7 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2-[(acetyloxy)methyl]-2-methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

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ΙT
     171868-39-6 189058-97-7 189059-19-6
     189059-57-2 189059-70-9 189059-84-5
     189059-85-6 189060-04-6 189060-07-9
     189060-10-4 189060-13-7 189060-21-7
     189060-33-1 189060-37-5 189060-45-5
     189060-48-8 383652-05-9 383652-11-7
     383652-22-0 383652-28-6 383652-33-3
     383652-38-8 383652-44-6 383652-50-4
     383652-66-2 383652-71-9 383652-76-4
     383652-81-1 383652-92-4 383652-98-0
     383654-76-0 383657-83-8
     RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (high-d. lipoprotein-cholesterol level elevating agents containing squalene
        synthase inhibitors)
RN
     171868-39-6 CAPLUS
     4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-
CN
     dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)
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RN 189058-97-7 CAPLUS CN \beta-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-
```

dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-19-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-N-[2-(1-pyrrolidinyl)ethyl]-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-57-2 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-1-(3-hydroxy-2,2-dimethylpropyl)-3-(1H-tetrazol-5-ylmethyl)-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189059-70-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-N-[2-(1-pyrrolidinyl)ethyl]-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-84-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-N-(methylsulfonyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189059-85-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[3-hydroxy-2-(hydroxymethyl)-2-methylpropyl]-N-(methylsulfonyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-04-6 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2-[(acetyloxy)methyl]-2-methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 189060-07-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 1-[3-(acetyloxy)-2-[(acetyloxy)methyl]-2-methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-N-(methylsulfonyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-10-4 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 189060-13-7 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-21-7 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-1-[3-hydroxy-2-(hydroxymethyl)-2-methylpropyl]-3-(1H-tetrazol-5-ylmethyl)-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189060-33-1 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2-[(acetyloxy)methyl]-2-methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-3-(1H-tetrazol-5-ylmethyl)-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-37-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[3-hydroxy-2-(hydroxymethyl)-2-methylpropyl]-2-oxo-N-[2-(1-pyrrolidinyl)ethyl]-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189060-45-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-N-(methylsulfonyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-48-8 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-3-(1H-tetrazol-5-ylmethyl)-, (3R,5S)-(9CI) (CA INDEX NAME)

RN 383652-05-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-N-(propylsulfonyl)-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-11-7 CAPLUS

CN D-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

RN 383652-22-0 CAPLUS

CN Butanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-28-6 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, trans- (9CI) (CA INDEX NAME)

RN 383652-33-3 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, trans- (9CI) (CA INDEX NAME)

.Absolute stereochemistry. Rotation (-).

RN 383652-38-8 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro- (9CI) (CA INDEX NAME)

RN 383652-44-6 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383652-50-4 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

RN 383652-66-2 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-71-9 CAPLUS

CN Benzenebutanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy- (9CI) (CA INDEX NAME)

RN 383652-76-4 CAPLUS

CN Benzenepentanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-81-1 CAPLUS

CN Benzenepentanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro-(9CI) (CA INDEX NAME)

RN 383652-92-4 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383652-98-0 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383654-76-0 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383657-83-8 CAPLUS

CN 2-Furancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/256,198

ANSWER 14 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:19789 CAPLUS

DOCUMENT NUMBER: 136:369691

TITLE: 4,1-Benzoxazepine derivatives as squalene synthase

inhibitors. 4. Microbial enantioselective ester hydrolysis for the preparation of optically active 4,1-benzoxazepine-3-acetic acid derivatives as

squalene synthase inhibitors

AUTHOR(S): Tarui, Naoki; Nakahama, Kazuo; Nagano, Yoichi; Izawa,

Motowo; Matsumoto, Kiyoharu; Kori, Masakuni; Nagata,

Toshiaki; Miki, Takashi; Yukimasa, Hidefumi

CORPORATE SOURCE: Pharmaceutical Research Division, Takeda Chemical

Industries, Ltd., Yodogawa-ku. Osaka, 532-8686, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (2002), 50(1),

59-65

CODEN: CPBTAL; ISSN: 0009-2363

PUBLISHER: Pharmaceutical Society of Japan DOCUMENT TYPE: Journal

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DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:369691

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AB Microbial enantioselective ester hydrolysis for the preparation of optically active (3R,5S)-(-)-5-phenyl-4,1- benzoxazepine-3-acetic acid derivs. as potent squalene synthase inhibitors was investigated. Pseudomonas diminuta and Pseudomonas taetrolens hydrolyzed the racemic Et ester of a 5-(2-chlorophenyl) analog to yield a (-)-carboxylic acid with excellent enantiomeric excess (>99% ee). The (-)-enantiomer was found to be an active inhibitor. Bulkiness of the ester moiety did not affect the enantioselectivity but did affect reactivity. The racemic Et esters of the 5-(2-methoxyphenyl) analog, 5-(2,3-dimethoxyphenyl) analog and 5-(2,4-dimethoxyphenyl) analog were also hydrolyzed with Pseudomonas taetrolens to afford enantiomerically pure (-)-carboxylic acids in large scale. As another route to (3R,5S)-(-)-7-chloro-5-(2,3-dimethoxyphenyl)-1neopentyl-2-oxo-1,2,3,5-tetrahydro-4,1-benzoxazepine-3-acetic acid (I), an earlier intermediate (-)-2-amino-5-chloro- α -(2,3dimethoxyphenyl) benzyl alc. was successfully obtained by asym. hydrolysis of (\pm) -5-chloro- α -(2,3-dimethoxyphenyl)-2-pivaloylaminobenzyl acetate with Pseudomonas sp. S-13 with >99% ee in kilogram scale followed by, alkaline treatment. The product was converted to I without racemization.

IT 171868-39-6P

RL: BPN (Biosynthetic preparation); PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (microbial enantioselective ester hydrolysis for the preparation of optically active 4,1-benzoxazepine-3-acetic acid derivs. as squalene synthase inhibitors)

RN 171868-39-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 177567-40-7P

RL: BPN (Biosynthetic preparation); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(microbial enantioselective ester hydrolysis for the preparation of optically active 4,1-benzoxazepine-3-acetic acid derivs. as squalene synthase inhibitors)

RN 177567-40-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester, (3R,5S)- (9CI) (CA INDEX NAME)

IT 152909-22-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(microbial enantioselective ester hydrolysis for the preparation of optically active 4,1-benzoxazepine-3-acetic acid derivs. as squalene synthase inhibitors)

RN 152909-22-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

REFERENCE COUNT:

23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/256,198

ANSWER 15 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:935587 CAPLUS

DOCUMENT NUMBER: 136:69829

TITLE: Preparation of dialkoxyphenyloxobenzoxazepineacetamide

squalene synthase inhibitors as antihyperlipidemic and

antihypercholesteremic agents

INVENTOR(S): Kori, Masakuni; Miki, Takashi; Nishimoto, Tomoyuki;

Tozawa, Ryuichi

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd, Japan

SOURCE: PCT Int. Appl., 643 pp.

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE: Patent English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA:	KIND DATE				APPLICATION NO.						DATE							
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OTHER SOURCE(S): MARPAT 136:69829

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AB Alkoxyphenyloxobenzoxazepineacetamides [I; R = (un)substituted 1-carboxyethyl, (un) substituted carboxyalkyl, sulfonylalkyl, (carboxycycloalkyl)alkyl, etc.; R1 = alkyl (un)substituted with alkanoyloxy or OH groups (if R = (un)substituted 1-carboxyethyl, alkyl, 4-carboxycyclohexylmethyl, or 4-carboxyphenylmethyl, then R1 must be substituted with a OH or alkanoyloxy group); R2 = lower alkyl; W = halogen] are prepared as squalene synthase inhibitors for the treatment of hyperlipidemia and the decrease of serum triglycerides and lipids. 4S)-I [R = Me(CH2)2SO2; R1 = HOCH2C(Me)2CH2; R2 = Me; W = Cl] (II) was prepared in 3 steps from hydroxyacid (III) by acetylation of the hydroxyl group with acetic anhydride, treatment of the acid with thionyl chloride in THF to generate the acid chloride in situ, and addition of the mixture to a solution of PrSO2NH2 in THF to provide the acetylated methoxyphenyloxobenzoxazepineacetamide I [R = PrSO2; R1 = AcOCH2C(Me)2CH2; R2 = Me; W = Cl]; hydrolysis of the acetoxy group with aqueous sodium hydroxide and ethanol provides II. Data for the inhibition of squalene synthase by I are given. Pharmaceutical compns. containing I [R = 3-(HO2CCH2CH2)C6H4; R1 = HOCH2CMe2CH2; R2 = Me; W = C1] are specified.

IT 383661-55-0P 383661-74-3P 383661-79-8P 383661-85-6P 383661-90-3P 383661-95-8P 383662-00-8P 383662-05-3P 383662-10-0P 383662-15-5P 383662-20-2P 383662-25-7P 383662-50-8P 383662-71-3P 383662-81-5P 383662-97-3P 383663-24-9P 383663-35-2P 383663-76-1P 383664-02-6P 383664-07-1P 383664-12-8P 383664-18-4P 383664-35-5P 383664-54-8P 383664-99-1P 383665-26-7P 383665-43-8P 383665-48-3P 383665-62-1P 383665-76-7P 383666-12-4P 383666-22-6P 383666-37-3P 383666-63-5P 383666-68-0P 383666-96-4P 383667-27-4P 383667-32-1P 383667-37-6P 383667-42-3P 383667-47-8P 383667-52-5P 383667-58-1P 383667-63-8P 383667-69-4P 383667-74-1P 383667-79-6P 383667-84-3P 383667-89-8P 383667-94-5P 383668-00-6P 383668-05-1P 383668-10-8P 383668-26-6P 383668-39-1P 383668-63-1P 383668-88-0P 383669-02-1P 383669-08-7P 383669-14-5P 383669-23-6P 383669-33-8P

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383669-42-9P 383669-51-0P 383669-66-7P
     383669-82-7P 383670-03-9P 383670-28-8P
     383670-38-0P 383670-49-3P 383670-59-5P
     383670-64-2P 383670-69-7P 383670-85-7P
     383671-02-1P 383671-23-6P 383671-45-2P
     383671-60-1P 383671-79-2P 383672-12-6P
     383672-25-1P 383672-30-8P 383672-35-3P
     383672-40-0P 383672-50-2P 383672-67-1P
     383672-82-0P 383672-88-6P 383672-95-5P
     383673-01-6P 383673-16-3P 383673-32-3P
     383673-59-4P 383673-75-4P 383674-10-0P
     383674-38-2P 383674-55-3P 383674-72-4P
     383674-89-3P 383674-95-1P 383675-11-4P
     383675-45-4P 383675-68-1P 383675-90-9P
     383676-16-2P 383676-57-1P 383676-81-1P
     383677-02-9P 383767-82-6P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (intermediates; preparation of dialkoxyphenyloxobenzoxazepineacetamide
        squalene synthase inhibitors as antihyperlipidemic and
        antihypercholesteremic agents)
RN
     383661-55-0 CAPLUS
CN
     4,1-Benzoxazepine-3-acetic acid, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-
     chloro-5-(2,3-dimethoxypheny1)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI)
     (CA INDEX NAME)
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Absolute stereochemistry. Rotation (-).

RN 383661-74-3 CAPLUS
CN L-Leucine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-,
ethyl ester (9CI) (CA INDEX NAME)

RN 383661-79-8 CAPLUS

CN D-Leucine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383661-85-6 CAPLUS

CN D-Leucine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 383661-90-3 CAPLUS

CN L-Methionine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383661-95-8 CAPLUS

CN D-Methionine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 383662-00-8 CAPLUS

CN D-Methionine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383662-05-3 CAPLUS

CN D-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 383662-10-0 CAPLUS

CN L-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383662-15-5 CAPLUS

CN D-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 383662-20-2 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, methyl ester, trans- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383662-25-7 CAPLUS

CN Cyclohexanepropanoic acid, α-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

RN 383662-50-8 CAPLUS

CN 3-Furancarboxylic acid, 2-[2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383662-71-3 CAPLUS

CN 2,4-Furandicarboxylic acid, 5-[2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]-, 2-ethyl 4-methyl ester (9CI) (CA INDEX NAME)

RN 383662-81-5 CAPLUS

CN 2-Furancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383662-97-3 CAPLUS

CN Benzeneacetic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 383663-24-9 CAPLUS

CN Benzenepropanoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383663-35-2 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383663-76-1 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383664-02-6 CAPLUS

CN Benzenepropanoic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 383664-07-1 CAPLUS

CN Benzoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383664-12-8 CAPLUS

CN Benzoic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methyl-, methyl ester (9CI) (CA INDEX NAME)

RN 383664-18-4 CAPLUS

CN Benzoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383664-35-5 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-ethoxy-, ethyl ester (9CI) (CA INDEX NAME)

RN 383664-54-8 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-(1-methylethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383664-99-1 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro-, ethyl ester (9CI) (CA INDEX NAME)

RN 383665-26-7 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383665-43-8 CAPLUS

CN Benzenepropanoic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-methoxy-, ethyl ester (9CI) (CA INDEX NAME)

RN 383665-48-3 CAPLUS

CN Benzeneacetic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383665-62-1 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383665-76-7 CAPLUS

CN Benzeneacetic acid, 4-[[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383666-12-4 CAPLUS

CN Benzenepropanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383666-22-6 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383666-37-3 CAPLUS

CN Benzenepropanoic acid, 3-[[((3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4,5-dimethoxy-, ethyl ester (9CI) (CA INDEX NAME)

RN 383666-63-5 CAPLUS

CN Benzenebutanoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383666-68-0 CAPLUS

CN Butanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 383666-96-4 CAPLUS

CN Benzenepropanoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-methyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383667-27-4 CAPLUS

CN Benzoic acid, 4-[[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 383667-32-1 CAPLUS

CN Propanoic acid, 2-[4-[2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]phenoxy]-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383667-37-6 CAPLUS

CN Acetic acid, [4-[2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]phenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383667-42-3 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383667-47-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383667-52-5 CAPLUS

CN Benzoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383667-58-1 CAPLUS

CN Benzoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 383667-63-8 CAPLUS

CN Benzoic acid, 2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383667-69-4 CAPLUS

CN 2-Thiophenecarboxylic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 383667-74-1 CAPLUS

CN 4-Thiazoleacetic acid, 2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383667-79-6 CAPLUS

CN 2-Furancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 383667-84-3 CAPLUS

CN Benzeneacetic acid, 4-[3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383667-89-8 CAPLUS

CN Benzoic acid, 4-[3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383667-94-5 CAPLUS

CN Benzoic acid, 3-[3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383668-00-6 CAPLUS

CN Benzoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy-, methyl ester (9CI) (CA INDEX NAME)

RN 383668-05-1 CAPLUS

CN Benzoic acid, 4-[2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383668-10-8 CAPLUS

CN Benzoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro-, methyl ester (9CI) (CA INDEX NAME)

RN 383668-26-6 CAPLUS

CN Benzenepentanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383668-39-1 CAPLUS

CN Benzeneacetic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy-, methyl ester (9CI) (CA INDEX NAME)

RN 383668-63-1 CAPLUS

CN Benzenebutanoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-methoxy-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383668-88-0 CAPLUS

CN Benzenebutanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383669-02-1 CAPLUS

CN 1-Naphthalenecarboxylic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-5,6,7,8-tetrahydro-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383669-08-7 CAPLUS

CN Butanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 383669-14-5 CAPLUS

CN Pentanoic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383669-23-6 CAPLUS

CN Hexanoic acid, 6-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 383669-33-8 CAPLUS

CN 3-Furancarboxylic acid, 2-[2-[[[(3S,5R)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 383669-42-9 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3S,5R)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383669-51-0 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3S,5R)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 383669-66-7 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-chloro-, methyl ester (9CI) (CA INDEX NAME)

RN 383669-82-7 CAPLUS

CN Benzenepropanoic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-(3-phenylpropoxy)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383670-03-9 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-(3-phenylpropoxy)-, ethyl ester (9CI) (CA INDEX NAME)

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RN 383670-28-8 CAPLUS

CN 1-Naphthalenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-5,6,7,8-tetrahydro-, ethyl ester (9CI) (CA INDEX NAME)

RN 383670-38-0 CAPLUS

CN 1-Naphthalenecarboxylic acid, 6-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383670-49-3 CAPLUS

CN 1-Naphthalenecarboxylic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383670-59-5 CAPLUS

CN 1-Naphthalenecarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383670-64-2 CAPLUS

CN Benzoic acid, 5-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)

RN 383670-69-7 CAPLUS

CN Benzoic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3yl]acetyl]amino]-2-fluoro-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN

383670-85-7 CAPLUS Acetic acid, [4-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-CN (2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3yl]acetyl]amino]phenoxy]difluoro-, ethyl ester (9CI) (CA INDEX NAME)

RN 383671-02-1 CAPLUS

CN Acetic acid, [3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]phenoxy]difluoro-, ethyl ester (9CI) (CA INDEX NAME)

.Absolute stereochemistry. Rotation (-).

RN 383671-23-6 CAPLUS

CN Benzenepropanoic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-fluoro-, methyl ester (9CI) (CA INDEX NAME)

RN 383671-45-2 CAPLUS

CN Benzenepentanoic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN

383671-60-1 CAPLUS Acetic acid, [4-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-CN (2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3yl]acetyl]amino]-3-fluorophenoxy]-, methyl ester (9CI) (CA INDEX NAME)

RN 383671-79-2 CAPLUS

CN Benzeneacetic acid, $3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy-<math>\alpha$, α -dimethyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383672-12-6 CAPLUS

CN Benzenebutanoic acid, $3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy-<math>\gamma$, γ -dimethyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 383672-25-1 CAPLUS

CN Benzenepentanoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-methoxy-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383672-30-8 CAPLUS

CN 2-Pyridinecarboxylic acid, 6-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383672-35-3 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383672-40-0 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383672-50-2 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383672-67-1 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383672-82-0 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (~).

RN 383672-88-6 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

RN 383672-95-5 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-phenyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383673-01-6 CAPLUS

CN 5-Thiazolebutanoic acid, 2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-(4-chlorophenyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 383673-16-3 CAPLUS

CN Acetic acid, [[5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-1H-benzimidazol-2-yl]thio]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383673-32-3 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-7-methoxy-, ethyl ester (9CI) (CA INDEX NAME)

RN 383673-59-4 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-7-ethoxy-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383673-75-4 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-7-propoxy-, methyl ester (9CI) (CA INDEX NAME)

RN 383674-10-0 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-7-(1-methylethoxy)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383674-38-2 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-methoxy-, ethyl ester (9CI) (CA INDEX NAME)

RN 383674-55-3 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-propoxy-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383674-72-4 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-(2-ethoxy-2-oxoethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

RN 383674-89-3 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-(1-methylethoxy)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383674-95-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383675-11-4 CAPLUS

CN Benzo[b]thiophene-2-carboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383675-45-4 CAPLUS

CN 2-Benzofuranpropanoic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 383675-68-1 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-methyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383675-90-9 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-7-methyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 383676-16-2 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-7-ethyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383676-57-1 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-7-propyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 383676-81-1 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4,6,7-trimethyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383677-02-9 CAPLUS

CN 2-Benzofurancarboxylic acid, 7-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-5-chloro-, ethyl ester (9CI) (CA INDEX NAME)

RN 383767-82-6 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 189060-51-3 383678-02-2

RL: RCT (Reactant); RACT (Reactant or reagent) (starting materials; preparation of dialkoxyphenyloxobenzoxazepineacetamide squalene synthase inhibitors as antihyperlipidemic and antihypercholesteremic agents)

RN 189060-51-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 383678-02-2 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-, (3S,5R)- (9CI) (CA INDEX NAME)

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TT 383652-33-3P 383652-44-6P 383652-56-0P 383652-66-2P 383652-92-4P 383652-98-0P 383653-04-1P 383653-14-3P 383653-20-1P 383653-31-4P 383653-40-5P 383653-71-2P 383654-03-3P 383654-14-6P 383654-54-4P 383654-65-7P 383654-88-4P 383655-31-0P 383655-09-2P 383655-19-4P 383655-31-0P 383655-93-4P 383655-52-5P 383655-73-0P 383655-93-4P 383656-68-6P 383656-78-8P 383656-90-4P 383657-01-0P 383657-12-3P 383657-22-5P 383657-38-3P 383657-61-2P 383657-72-5P 383657-83-8P 383657-94-1P 383658-05-7P 383658-15-9P
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383658-25-1P 383658-36-4P 383658-46-6P 383658-84-2P 383658-95-5P 383659-31-2P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(title compds.; preparation of dialkoxyphenyloxobenzoxazepineacetamide squalene synthase inhibitors as antihyperlipidemic and antihypercholesteremic agents)

RN 383652-33-3 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, trans- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-44-6 CAPLUS

CN Benzenepropanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

RN 383652-56-0 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383652-66-2 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-92-4 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro-(9CI) (CA INDEX NAME)

RN 383652-98-0 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383653-04-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-N-(propylsulfonyl)-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 383653-14-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, N-(butylsulfonyl)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383653-20-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-N-[[3-(acetyloxy)propyl]sulfonyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 383653-31-4 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-N-[[3-(phenylthio)propyl]sulfonyl]-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383653-40-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-N-[[3-(2-pyridinylthio)propyl]sulfonyl]-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 383653-71-2 CAPLUS

CN D-Leucine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383654-03-3 CAPLUS

CN L-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

RN 383654-14-6 CAPLUS

CN D-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383654-54-4 CAPLUS

CN Benzeneacetic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383654-65-7 CAPLUS

CN Benzenepropanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383654-88-4 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

RN 383654-99-7 CAPLUS

CN Benzenepropanoic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383655-09-2 CAPLUS

CN Benzoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

RN 383655-19-4 CAPLUS

CN Benzoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383655-31-0 CAPLUS

CN Benzoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-methyl- (9CI) (CA INDEX NAME)

RN 383655-41-2 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-ethoxy-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383655-52-5 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-(1-methylethoxy)- (9CI) (CA INDEX NAME)

RN 383655-73-0 CAPLUS

CN Benzenepropanoic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383655-93-4 CAPLUS

CN Benzeneacetic acid, 4-[[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]- (9CI) (CA INDEX NAME)

$$MeO$$
 MeO
 MeO
 R
 HO_2C
 HO
 Me
 Me

RN 383656-19-7 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4,5-dimethoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383656-30-2 CAPLUS

CN Benzenebutanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383656-42-6 CAPLUS

CN Benzenepropanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383656-68-6 CAPLUS

CN Benzenepropanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-methoxy- (9CI) (CA INDEX NAME)

RN 383656-78-8 CAPLUS

CN Benzoic acid, 4-[[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383656-90-4 CAPLUS

CN Propanoic acid, 2-[4-[2-[[[(3R,5s)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 383657-01-0 CAPLUS

CN Acetic acid, [4-[2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]phenoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383657-12-3 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383657-22-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383657-38-3 CAPLUS

CN Benzoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383657-50-9 CAPLUS

CN Benzoic acid, 2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383657-61-2 CAPLUS

CN 2-Thiophenecarboxylic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383657-72-5 CAPLUS

CN 4-Thiazoleacetic acid, 2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383657-83-8 CAPLUS

CN 2-Furancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383657-94-1 CAPLUS

CN Benzeneacetic acid, 4-[3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383658-05-7 CAPLUS

CN Benzoic acid, 4-[3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]- (9CI) (CA INDEX NAME)

RN 383658-15-9 CAPLUS

CN Benzoic acid, 3-[3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383658-25-1 CAPLUS

CN Benzoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy- (9CI) (CA INDEX NAME)

RN 383658-36-4 CAPLUS

CN Benzoic acid, 4-[2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383658-46-6 CAPLUS

CN Benzoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro-(9CI) (CA INDEX NAME)

RN 383658-84-2 CAPLUS

CN Pentanoic acid, 5-[[[(3R,5s)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383658-95-5 CAPLUS

CN Hexanoic acid, 6-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383659-31-2 CAPLUS

CN Benzenepropanoic acid, 4-chloro-3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

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TT 383652-05-9P 383652-11-7P 383652-16-2P 383652-22-0P 383652-28-6P 383652-38-8P 383652-50-4P 383652-61-7P 383652-71-9P 383652-76-4P 383652-81-1P 383652-87-7P 383653-09-6P 383653-25-6P 383653-35-8P 383653-45-0P 383653-86-5P 383653-92-7P 383653-97-2P 383653-97-2P 383654-20-4P 383654-25-9P 383654-20-4P 383654-25-9P 383654-46-4P 383654-60-2P 383654-70-4P 383654-76-0P 383654-82-8P 383655-25-2P 383655-36-5P 383655-46-7P 383655-57-0P 383655-78-5P 383655-83-2P
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383655-98-9P 383656-06-2P 383656-24-4P
     383656-36-8P 383656-63-1P 383656-73-3P
     383656-84-6P 383656-95-9P 383657-07-6P
     383657-17-8P 383657-27-0P 383657-32-7P
     383657-44-1P 383657-55-4P 383657-67-8P
     383657-78-1P 383657-89-4P 383657-99-6P
     383658-10-4P 383658-20-6P 383658-30-8P
     383658-40-0P 383658-51-3P 383658-57-9P
     383658-62-6P 383658-68-2P 383658-74-0P
     383658-79-5P 383658-90-0P 383659-00-5P
     383659-06-1P 383659-21-0P 383659-26-5P
     383659-37-8P 383659-42-5P 383659-48-1P
     383659-55-0P 383659-61-8P 383659-67-4P
     383659-73-2P 383659-79-8P 383659-84-5P
     383659-89-0P 383659-94-7P 383659-99-2P
     383660-05-7P 383660-11-5P 383660-16-0P
     383660-21-7P 383660-26-2P 383660-32-0P
     383660-38-6P 383660-43-3P 383660-48-8P
     383660-52-4P 383660-57-9P 383660-62-6P
     383660-67-1P 383660-72-8P 383660-77-3P
     383660-82-0P 383660-87-5P 383660-93-3P
     383660-98-8P 383661-03-8P 383661-08-3P
     383661-12-9P 383661-17-4P 383661-22-1P
     383661-27-6P 383661-31-2P 383661-36-7P
     383661-40-3P 383661-45-8P 383661-50-5P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (title compds.; preparation of dialkoxyphenyloxobenzoxazepineacetamide
        squalene synthase inhibitors as antihyperlipidemic and
        antihypercholesteremic agents)
RN
     383652-05-9 CAPLUS
     4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-
CN
     tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-N-(propylsulfonyl)-,
     (3R,5S) - (9CI) (CA INDEX NAME)
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RN 383652-11-7 CAPLUS
CN D-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-
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dimethylpropy1)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl](9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-16-2 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383652-22-0 CAPLUS

CN Butanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383652-28-6 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, trans- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-38-8 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro-(9CI) (CA INDEX NAME)

RN 383652-50-4 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383652-61-7 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 383652-71-9 CAPLUS

CN Benzenebutanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-76-4 CAPLUS

CN Benzenepentanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy-(9CI) (CA INDEX NAME)

RN 383652-81-1 CAPLUS

CN Benzenepentanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383652-87-7 CAPLUS

CN 3-Furancarboxylic acid, 2-[2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 383653-09-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-N-(butylsulfonyl)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383653-25-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-N-[(3-hydroxypropyl)sulfonyl]-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 383653-35-8 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-N-[[3-(phenylthio)propyl]sulfonyl]-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383653-45-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-N-[[3-(2-pyridinylthio)propyl]sulfonyl]-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 383653-66-5 CAPLUS

CN L-Leucine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383653-76-7 CAPLUS

CN D-Leucine, N-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 383653-81-4 CAPLUS

CN D-Leucine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383653-86-9 CAPLUS

CN L-Methionine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 383653-92-7 CAPLUS

CN D-Methionine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383653-97-2 CAPLUS

CN D-Methionine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

RN 383654-09-9 CAPLUS

CN L-Alanine, N-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383654-20-4 CAPLUS

CN D-Alanine, N-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 383654-25-9 CAPLUS

CN Cyclohexanepropanoic acid, $\alpha-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, (<math>\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383654-30-6 CAPLUS

CN 3-Furancarboxylic acid, 2-[2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 383654-36-2 CAPLUS

CN 2,4-Furandicarboxylic acid, 5-[2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383654-41-9 CAPLUS

CN 2-Furancarboxylic acid, 5-[[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 383654-46-4 CAPLUS

CN 2-Furancarboxylic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383654-60-2 CAPLUS

CN Benzeneacetic acid, 4-[[['(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383654-70-4 CAPLUS

CN Benzenepropanoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383654-76-0 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383654-82-8 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383654-94-2 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

RN 383655-04-7 CAPLUS

CN Benzenepropanoic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383655-14-9 CAPLUS

CN Benzoic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

RN 383655-25-2 CAPLUS

CN Benzoic acid, 3-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383655-36-5 CAPLUS

CN Benzoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-methyl- (9CI) (CA INDEX NAME)

RN 383655-46-7 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-ethoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383655-57-0 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-(1-methylethoxy)- (9CI) (CA INDEX NAME)

RN 383655-78-5 CAPLUS

CN Benzenepropanoic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 383655-83-2 CAPLUS

CN Benzeneacetic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383655-98-9 CAPLUS

CN Benzeneacetic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$MeO$$
 MeO
 MeO
 R
 HO_2C
 AcO
 Me
 Me

RN 383656-06-2 CAPLUS

CN Benzenepropanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]- (9CI) (CA INDEX NAME)

$$MeO$$
 MeO
 MeO
 R
 HO_2C
 HO
 Me
 Me

RN 383656-24-4 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4,5-dimethoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383656-36-8 CAPLUS

CN Benzenebutanoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383656-63-1 CAPLUS

CN Benzenepropanoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383656-73-3 CAPLUS

CN Benzenepropanoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-methoxy- (9CI) (CA INDEX NAME)

RN 383656-84-6 CAPLUS

CN Benzoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$MeO$$
 MeO
 R
 HO_2C
 R
 MeO
 R
 MeO

RN 383656-95-9 CAPLUS

CN Propanoic acid, 2-[4-[2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]phenoxy]-2-methyl- (9CI) (CA INDEX NAME)

RN 383657-07-6 CAPLUS

CN Acetic acid, [4-[2-[[((3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]phenoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383657-17-8 CAPLUŠ

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383657-27-0 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383657-32-7 CAPLUS

CN Benzoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383657-44-1 CAPLUS

CN Benzoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383657-55-4 CAPLUS

CN Benzoic acid, 2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383657-67-8 CAPLUS

CN 2-Thiophenecarboxylic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383657-78-1 CAPLUS

CN 4-Thiazoleacetic acid, 2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383657-89-4 CAPLUS

CN 2-Furancarboxylic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383657-99-6 CAPLUS

CN Benzeneacetic acid, 4-[3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]- (9CI) (CA INDEX NAME)

RN 383658-10-4 CAPLUS

CN Benzoic acid, 4-[3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383658-20-6 CAPLUS

CN Benzoic acid, 3-[3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]propoxy]- (9CI) (CA INDEX NAME)

RN 383658-30-8 CAPLUS

CN Benzoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383658-40-0 CAPLUS

CN Benzoic acid, 4-[2-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 383658-51-3 CAPLUS

CN Benzoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383658-57-9 CAPLUS

CN Benzeneacetic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy- (9CI) (CA INDEX NAME)

RN 383658-62-6 CAPLUS

CN Benzenebutanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383658-68-2 CAPLUS

CN 1-Naphthalenecarboxylic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-5,6,7,8-tetrahydro-(9CI) (CA INDEX NAME)

RN 383658-74-0 CAPLUS

CN Butanoic acid, 4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383658-79-5 CAPLUS

CN Butanoic acid, 4-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383658-90-0 CAPLUS

CN Pentanoic acid, 5-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383659-00-5 CAPLUS

CN Hexanoic acid, 6-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383659-06-1 CAPLUS

CN 3-Furancarboxylic acid, 2-[2-[[[(3S,5R)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 383659-21-0 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3S,5R)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383659-26-5 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3S,5R)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-fluoro-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 383659-37-8 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-chloro-(9CI) (CA INDEX NAME)

RN 383659-42-5 CAPLUS

CN Benzenepropanoic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-(3-phenylpropoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383659-48-1 CAPLUS

CN Benzenepropanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-(3-phenylpropoxy)- (9CI) (CA INDEX NAME)

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RN 383659-55-0 CAPLUS

CN 1-Naphthalenepropanoic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-5,6,7,8-tetrahydro-(9CI) (CA INDEX NAME)

RN 383659-61-8 CAPLUS

CN 1-Naphthalenecarboxylic acid, 6-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383659-67-4 CAPLUS

CN 1-Naphthalenecarboxylic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383659-73-2 CAPLUS

CN 1-Naphthalenecarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383659-79-8 CAPLUS

CN Benzoic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

RN 383659-84-5 CAPLUS

CN Benzoic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-fluoro-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383659-89-0 CAPLUS

CN Acetic acid, [4-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]phenoxy]difluoro-(9CI) (CA INDEX NAME)

RN 383659-94-7 CAPLUS

CN Acetic acid, [3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]phenoxy]difluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383659-99-2 CAPLUS

CN Benzenepropanoic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-2-fluoro- (9CI) (CA INDEX NAME)

RN 383660-05-7 CAPLUS

CN Benzenepentanoic acid, 3-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$MeO$$
 MeO
 MeO
 MeO
 NH
 O
 R
 NH
 O
 Me
 NH
 O
 Me
 NH
 O
 Me
 Me

RN 383660-11-5 CAPLUS

CN Acetic acid, [4-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-fluorophenoxy]- (9CI) (CA INDEX NAME)

RN 383660-16-0 CAPLUS

CN Benzeneacetic acid, 3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3yl]acetyl]amino]-4-methoxy-α,α-dimethyl- (9CI) (CA INDEX
NAME)

Absolute stereochemistry. Rotation (-).

RN 383660-21-7 CAPLUS

CN Benzenebutanoic acid, $3-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methoxy-<math>\gamma$, γ -dimethyl- (9CI) (CA INDEX NAME)

RN 383660-26-2 CAPLUS

CN 2-Pyridinecarboxylic acid, 6-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383660-32-0 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383660-38-6 CAPLUS

CN 4-Thiazolecarboxylic acid, 2-[[((3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383660-43-3 CAPLUS

CN 5-Thiazoleacetic acid, 2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383660-48-8 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383660-52-4 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

RN 383660-57-9 CAPLUS

CN 5-Thiazolepropanoic acid, 2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383660-62-6 CAPLUS

CN 5-Thiazolebutanoic acid, 2-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4-(4-chlorophenyl)- (9CI) (CA INDEX NAME)

RN 383660-67-1 CAPLUS

CN Acetic acid, [[5-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-1H-benzimidazol-2-yl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383660-72-8 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-7-methoxy- (9CI) (CA INDEX NAME)

RN 383660-77-3 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-7-ethoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383660-82-0 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-7-propoxy- (9CI) (CA INDEX NAME)

RN 383660-87-5 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-7-(1-methylethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383660-93-3 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-methoxy- (9CI) (CA INDEX NAME)

RN 383660-98-8 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-propoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383661-03-8 CAPLUS

CN 2-Benzofurancarboxylic acid, 3-(carboxymethoxy)-5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383661-08-3 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-(1-methylethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383661-12-9 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383661-17-4 CAPLUS

CN Benzo[b]thiophene-2-carboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383661-22-1 CAPLUS

CN 2-Benzofuranpropanoic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

RN 383661-27-6 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383661-31-2 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-7-methyl- (9CI) (CA INDEX NAME)

RN 383661-36-7 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-7-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383661-40-3 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-7-propyl- (9CI) (CA INDEX NAME)

RN 383661-45-8 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-4,6,7-trimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 383661-50-5 CAPLUS

CN 2-Benzofurancarboxylic acid, 5-chloro-7-[[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/256,198

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ACSESSION NUMBER: 2001:932483 CAPLUS

DOCUMENT NUMBER: 136:50294

TITLE: Drug design of squalene synthase inhibitors by X-ray

structure computer analysis

INVENTOR(S): Usui, Hiroyuki; Katakura, Shinichi; Suzuki, Makoto

PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 131 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
		1				
JP 2001354587	A2	20011225	JP 2000-177413	20000613		
PRIORITY APPLN. INFO.:			JP 2000-177413	20000613		
GI						

AB A method for designing inhibitors of squalene synthase by computer anal. of X-ray crystallog. structure of the enzyme complexed with the known inhibitors, is disclosed. Divalent metal ion binding or hydrogen bonding by the carboxyl groups of Asp80, Glu83, and Asp84, or Asp219, Glu222, and Asp223, are used for inhibition. The compds. having the general structure I (Ar = possibly substituted single or double aromatic ring, R1 = single or double ring aromatic heterocycle, possibly substituted with single or double ring aromatic heterocycle, or C2-C6 alkenyl, A1 and A2 = C, O, S, CH, CR2, CH2, CHR3, C=0, NH, or NR4 (R2, R3, and R4 = C1-C6 alkyl)) or II (R1, A1, A2, same as above, B and Y = C, O, S, CH, CR2, CH2, CHR3, C=O, NH, or NR4 (R2, R3, and R4 = C1-C6 alkyl)), as preventive or therapeutic agent for hypercholesterolemia are claimed. Crystals of the complex of the soluble domain of squalene synthase (amino acid residues 31-370) with previously known inhibitors, D-61-7267 (III) (WO 9829380) and D-91-1169 (IV) (JP 09186880) were obtained and the three dimensional structures were determined Hydrophobic van der Waals interactions between naphthalene rings A and B of III, or benzene ring A of IV, and hydrophobic amino acids, Val179, Leu183, Met207, Gly208, Leu211, Tyr276, Phe288, and Pro292 was detected. Likewise, interactions between naphthalene rings C and D of III, or benzene ring B of IV, and hydrophobic amino acids Phe54, Val69, Phe72, Tyr73, Leu76, Val179, Leu183, and Phe288, were observed

IT 189058-86-4, D 91-1169

RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(drug design of squalene synthase inhibitors by x-ray structure

computer anal.)

RN 189058-86-4 CAPLUS

CN L-Aspartic acid, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

10/256,198

ANSWER 17 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

Accession number: 2001:900250 Caplus

DOCUMENT NUMBER: 136:272650

TITLE: Novel 4,1-benzoxazepine derivatives with potent

squalene synthase inhibitory activities

AUTHOR(S): Miki, Takashi; Kori, Masakuni; Mabuchi, Hiroshi;

Banno, Hiroshi; Tozawa, Ryu-ichi; Nakamura, Masahira;

Itokawa, Shigekazu; Sugiyama, Yasuo; Yukimasa,

Hidefumi

CORPORATE SOURCE: Pharmaceutical Research Division, Takeda Chemical

Industries, Ltd., Yodogawa-ku, Juso-Honmachi, Osaka,

(2001)

Volume Date

532-8686, Japan

SOURCE: Bioorganic & Medicinal Chemistry

2002, 10(2), 401-414

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:272650

GI

Ι

AB A series of (3,5-trans)-2-oxo-5-phenyl-1,2,3,5-tetrahydro-4,1benzoxazepine derivs. were synthesized and evaluated for squalene synthase inhibitory and cholesterol biosynthesis inhibitory activities. Through modification of substituents of the lead compds., it was found that 4,1-benzoxazepine-3-acetic acid derivs. with iso-Bu and neopentyl groups at the 1-position, the chloro atom at the 7-position, and the chloro and methoxy groups at the 2'-position on the 5-Ph ring, had potent squalene synthase inhibitory activity. Among such compds., the 5-(2,3-dimethoxyphenyl) derivative I exhibited potent inhibition of cholesterol biosynthesis in HepG2 cells. As a result of optical resolution study of I, the absolute stereochem. required for inhibitory activity was determined to be 3R,5S. In vivo study showed that the sodium salt of (3R, 5S) - 7-chloro-5-(2, 3-dimethoxyphenyl)-1-neopentyl-2-oxo-1,2,3,5tetrahydro-4,1-benzoxazepine-3-acetic acid effectively reduced plasma cholesterol in marmosets.

IT 152909-46-1P 171868-38-5P 171868-39-6P 171962-07-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzoxazepine derivs. with potent squalene synthase inhibitory activities)

RN 152909-46-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 171868-38-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 171868-39-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 171962-07-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, sodium salt, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Na

IT 152909-22-3P 406684-80-8P 406684-81-9P 736155-92-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzoxazepine derivs. with potent squalene synthase inhibitory activities)

RN 152909-22-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

RN 406684-80-8 CAPLUS
CN L-Leucine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 406684-81-9 CAPLUS
CN L-Leucine, N-[[(3S,5R)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 736155-92-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, methyl ester, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

20

REFERENCE COUNT:

THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 18 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:416879 CAPLUS

DOCUMENT NUMBER: 135:19434

TITLE: Process for production of optically active benzhydrols

by asymmetric hydrogenation of benzophenone

derivatives

INVENTOR(S): Yamano, Toru; Oi, Satoru; Yamashita, Masayuki

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 49 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	PATENT NO.					KIND DATE					ICAT:	ION I		DATE			
											- -						
WO	WO 2001040162				A1 (20010607) W					WO 2	000-	JP83:		20001129			
	W:	ΑE,	AG,	AL,	AM,	AU,	AZL	BA/	BB,	BG,	BR,	BY,	ΒZ,	CA,	CN,	CR,	CU,
		CZ,	DM,	DZ,	EE,	GD,	GE,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KG,	KR,	KZ,
		LC,	LK,	LR,	LT,	LV,	MA,	MD,	MG,	MK,	MN,	MX,	NO,	NZ,	PL,	RO,	RU,
		SG,	SI,	SK,	ТJ,	TM,	TR,	TT,	UA,	US,	UZ,	VN,	YU,	ZA,	AM,	AZ,	BY,
		KG,	ΚZ,	MD,	RU,	TJ,	TM										
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	ŬĠ,	ZW,	AT,	BE,	CH,	CY,
		DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,
		ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG		
JP 2001220371					A2 20010814					JP 2000-362780					20001129		
PRIORITY APPLN. INFO.:									JP 1999-341015				1	A 19	9991	130	
OTHER SOURCE(S):				CASI	CASREACT 135:19434; MARPAT 135:19434												
GI																	

AR A process for production of optically active compds. of general formula (I) [wherein R1 and R2 are each hydrogen or (un)substituted hydrocarbyl or acyl; ring A or B represents (un) substituted benzene ring; * represents an asym. carbon atom] is characterized by hydrogenating a benzophenone compound of general formula (II; R1 and R2 are same above) in the presence of both an optically active ruthenium-phosphine-amine complex prepared through isolation from a phosphine represented by, e.g., the general formula PR3R4R5 (wherein R3, R4 and R5 are each optionally substituted hydrocarbyl or R3 and R4 are linked together to form a cyclic hydrocarbyl ring), an amine of the general formula NHR8R9 [wherein R8 and R9 are each hydrogen or (un)substituted hydrocarbyl] and a ruthenium complex, and a base. This process efficiently gives optically active benzhydrols, which are useful as intermediates for drugs such as squalene synthetase inhibitors and triglyceride-lowering agents, in high yields under mild conditions at low hydrogen pressure and near room temperature Thus, 292 mg (2-amino-5chlorophenyl) (2,3-dimethoxyphenyl) methanone and 24 mg [RuCl2[(R)xylBINAP]][(R)-daipen] [xyl-BINAP = 2,2'-bis(dicyclohexylphosphino)-6,6'-

dimethyl-1,1'-biphenyl, daipen = 1-isopropyl-2,2-bis(pmethoxyphenyl)ethlylenediamine] (REG 220114-32-9) were added to a glass
autoclave, followed by purging the autoclave with Ar and adding a solution of
0.03 mL 1.0 M Me3COK/Me3COH and 2 mL toluene which had been purged with
Ar, and the resulting mixture was purged with Ar and stirred at room
temperature

under hydrogen pressure of 7 atm to give 97.1% (S)-(2-amino-5-chlorophenyl)(2,3-dimethoxyphenyl)methanol (98.7% e.e.). The latter compound was converted in 8 steps into N-[(3R,5S)-1-(3-acetoxy-2,2-dimethylpropyl)-7-chloro-5-(2,3-dimethoxyphenyl)-2-oxo-1,2,3,5-tetrahydro-4,1-benzoxazepine-3-acetyl]piperidine-4-acetic acid which is a known squalene synthetase inhibitor.

IT 189059-61-8P 189059-65-2P 189059-71-0P 189060-51-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(process for production of optically active benzhydrols by asym. hydrogenation of benzophenone derivs. in presence of optically active ruthenium phosphine amine complex)

RN 189059-61-8 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-, ethyl ester, (3R,5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-65-2 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 189059-71-0 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-51-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

IT 189060-13-7P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(process for production of optically active benzhydrols by asym. hydrogenation of benzophenone derivs. in presence of optically active ruthenium phosphine amine complex)

RN 189060-13-7 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 19 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

DOCUMENT NUMBER: 134:252365

TITLE: Preparation of oxazinobenzoxazepineacetates and

2001:224390 CAPLUS

analogs as squalene synthetase inhibitors

INVENTOR(S): Hayward, Cheryl M.; Scully, Douglas A.

PATENT ASSIGNEE(S): Pfizer Inc., USA SOURCE: U.S., 44 pp.

U.S., 44 pp. CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

F	PATENT NO.	KIND	DATE	API	PLICATION NO.	DATE		
_								
τ	JS 6207664	B1	20010327	US	1999-441339		19991116	
PRIORI	TY APPLN. INFO.:			US	1998-109939P	Ρ	19981125	
OTHER	SOURCE(S):	MARPAT	134:252365					
GI								

$$R^1$$
 R
 Z^1
 R^3
 R^2
 Z
 R^4
 R^3

AB Title compds. [I; R = (un)substituted Ph or -naphthyl; R1,R2 = H, halo, alkyl, alkoxy, etc.; R3 = CO2H, alkoxycarbonyl, CONH2, etc.; R4 = alk(en)yl, cycloalkylmethyl, Ph, etc.; Z = O, S, CH2; Z1 = O or S] were prepared (no data). Thus, (1R,7S,9R)-I [R = C6H3(OMe)2-2,3, R1 = 5-Me, R2 = H, R3 = CO2H, R4 = CMe3, Z1 = Z2 = O] was prepared starting from 3-tert-butyl-7-methyl-3,4-dihydro-2H-1,4-benzoxazine and 2,3-(MeO)2C6H3CHO.

IT 331634-15-2P 331634-23-2P 331634-31-2P 331634-57-2P 331634-58-3P 331634-77-6P 331634-78-7P 331635-12-2P 331635-14-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of oxazinobenzoxazepineacetates and analogs as squalene synthetase inhibitors)

RN 331634-15-2 CAPLUS

CN 8H-1,4-Oxazino[2,3,4-jk][4,1]benzoxazepine-6-acetic acid, 10-chloro-8-(2,3-dimethoxyphenyl)-3-(1,1-dimethylethyl)-2,3,5,6-tetrahydro-5-oxo-, (3R,6R,8S)-rel- (9CI) (CA INDEX NAME)

RN 331634-23-2 CAPLUS

CN 1H,6H-Pyrido[3,2,1-jk][4,1]benzoxazepine-3-acetic acid, 10-chloro-1-(2,3-dimethoxyphenyl)-6-(1,1-dimethylethyl)-3,4,7,8-tetrahydro-4-oxo-, (1R,3S,6R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 331634-31-2 CAPLUS

CN 1H,6H-Pyrido[3,2,1-jk][4,1]benzoxazepine-3-acetic acid, 10-chloro-1-(2,3-dimethoxyphenyl)-3,4,7,8-tetrahydro-6-(1-methylethyl)-4-oxo-, (1R,3S,6R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 331634-57-2 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[(1R,3S,6R)-10-chloro-1-(2,3-dimethoxyphenyl)-6-(1,1-dimethylethyl)-3,4,7,8-tetrahydro-4-oxo-1H,6H-pyrido[3,2,1-jk][4,1]benzoxazepin-3-yl]acetyl]-, rel- (9CI) (CA INDEX

NAME)

Relative stereochemistry.

RN 331634-58-3 CAPLUS

CN 3-Piperidinecarboxylic acid, 1-[[(1R,3S,6R)-10-chloro-1-(2,3-dimethoxyphenyl)-6-(1,1-dimethylethyl)-3,4,7,8-tetrahydro-4-oxo-1H,6H-pyrido[3,2,1-jk][4,1]benzoxazepin-3-yl]acetyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 331634-77-6 CAPLUS

CN 3-Piperidinecarboxylic acid, 1-[[(1R,3S,6R)-10-chloro-1-(2,3-dimethoxyphenyl)-3,4,7,8-tetrahydro-6-(1-methylethyl)-4-oxo-1H,6H-pyrido[3,2,1-jk][4,1]benzoxazepin-3-yl]acetyl]-, rel- (9CI) (CA INDEX NAME)

RN 331634-78-7 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[(1R,3S,6R)-10-chloro-1-(2,3-dimethoxyphenyl)-3,4,7,8-tetrahydro-6-(1-methylethyl)-4-oxo-1H,6H-pyrido[3,2,1-jk][4,1]benzoxazepin-3-yl]acetyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 331635-12-2 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[(3R,6R,8S)-10-chloro-8-(2,3-dimethoxyphenyl)-3-(1,1-dimethylethyl)-2,3,5,6-tetrahydro-5-oxo-8H-1,4-oxazino[2,3,4-jk][4,1]benzoxazepin-6-yl]acetyl]-, rel- (9CI) (CA INDEX NAME)

RN 331635-14-4 CAPLUS

CN 3-Piperidinecarboxylic acid, 1-[[(3R,6R,8S)-10-chloro-8-(2,3-dimethoxyphenyl)-3-(1,1-dimethylethyl)-2,3,5,6-tetrahydro-5-oxo-8H-1,4-oxazino[2,3,4-jk][4,1]benzoxazepin-6-yl]acetyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

REFERENCE COUNT:

10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/256,198

L4 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1998:180583 CAPLUS

DOCUMENT NUMBER:

128:230397

TITLE:

Preparation of 4,1-benzoxazepin-2-one derivatives and

their uses

INVENTOR(S):

Yukimasa, Hidefumi; Tozawa, Ryuichi; Kori, Masakuni;

Kitano, Kazuaki; Sugiyama, Yasuo

PATENT ASSIGNEE(S):

Takeda Chemical Industries, Ltd., Japan

SOURCE:

U.S., 105 pp., Cont.-in-part of U.S. Ser. No. 195,131,

abandoned.
CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE			
US 5726306 US 5885979 PRIORITY APPLN. INFO.:	A A	19980310 19990323	US 1994-338163 US 1997-852292 JP 1992-99541 JP 1992-339947 US 1993-49455 US 1994-195131 JP 1994-244136 US 1994-338163	B1 B2 A	19941109 19970507 19920420 19921221 19930420 19940209 19941007 19941109		

OTHER SOURCE(S):

MARPAT 128:230397

GI

$$\begin{array}{c|c}
R^2 & R^3 \\
 & O \\
 & N \\
 & N \\
 & R^1 \\
 & I
\end{array}$$

AB Title compds. I (R = halogen; R1 = H, benzyl, alkyl, alkynyl, etc.; R2 = H, alkyl, Ph, heterocyclic, etc.; R3 = H, alkyl, Ph, heterocyclic, etc.; X = bond, spacer with chain length of 1-7 atoms; Y = carboxyl, alkoxy carbonyl, hydroxyl, amino group, Ph, carbamoyl group, etc.) and salts are prepared from condensation of II with 5-oxo-tetrahydro-2-furancarbonyl chloride and ClCO(Z)nCOOR4 ((Z)n = (CH2)3, CHCl(CH2)2, trans-CH:CH, etc.;

R4 = H, Et, etc.). Title compds. I are useful for inhibiting squalene synthetase and fungal growth, and which are useful for treating or preventing hyperlipidemia in oral tablets or injections.

IT 171868-39-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of benzoxazepinone derivs. and their uses)

RN 171868-39-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 171868-38-5P 171962-07-5P 204585-86-4P 204586-14-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzoxazepinone derivs. and their uses)

RN 171868-38-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 171962-07-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, sodium salt, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Na

RN 204585-86-4 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 204586-14-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-(9CI) (CA INDEX NAME)

IT 171768-62-0P 171768-63-1P 171868-45-4P 171868-46-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzoxazepinone derivs. and their uses)

RN 171768-62-0 CAPLUS

CN L-Alanine, N-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, 1,1-dimethylethyl ester, (3S-trans)- (9CI) (CA INDEX NAME)

RN 171768-63-1 CAPLUS

CN L-Alanine, N-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3S-trans)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 171868-45-4 CAPLUS

CN L-Alanine, N-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, 1,1-dimethylethyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

RN 171868-46-5 CAPLUS

CN L-Alanine, N-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

7

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:31309 CAPLUS

DOCUMENT NUMBER:

128:102107

TITLE:

Preparation of 4,1-benzoxazepines and

4,1-benzothiazepines and their use as squalene

synthetase inhibitors

INVENTOR(S):

Hamanaka, Ernest Seiichi; Hayward, Cheryl Myers

PATENT ASSIGNEE(S): Pfizer Inc., USA

SOURCE:

PCT Int. Appl., 141 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.					KIND DATE				APPL	ICAT:		DATE					
	WO	WO 9748701			A1 19971224				1	WO 1	997-:	IB55	19970514					
		W:	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,
			DK,	EE,	ES,	FI,	GB,	GE,	HU,	IL,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,
			LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,
			RO,	RU,	SD,	SE,	SG,	SI,	SK,	ТJ,	TM,	TR,	TT,	UA,	UG,	US,	UZ,	VN,
			ΥU,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM						
		RW:	GH,	KE,	LS,	MW,	SD,	SZ,	UG,	AT,	BE,	CH,	DE,	DK,	ES,	FI,	FR,	GB,
			GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,
			ML,	MR,	ΝE,	SN,	TD,	TG										
AU 9724016			A1 19980107				AU 1997-24016					19970514						
	US	6537	987			В1		2003	0325	1	US 1	998-	2021	06		1	9981	218
PRIORITY APPLN. INFO.:						US 1996-22365P					:	P 19960620						
							WO 1997-IB550					Ţ	W 1	9970	514			

OTHER SOURCE(S): MARPAT 128:102107

GΙ

AB The invention relates to certain benzoxazepinones and benzothiazepinones I and their pharmaceutically acceptable cationic and anionic salts, prodrugs, and stereoisomers [wherein X = O, S, S(O), or S(O)2; Y = CO or CH2; T = 4- to 7-membered mono-aza saturated heterocycle bound at N, optionally containing thio or oxo and optionally monosubstituted on C with OH, C1-4 alkoxy, or CO2H; Z = CO2H or derivs., including tetrazol-5-yl; Z1 =H, CO2H, OH, alkoxy, alkoxycarbonyl; R1, R2 = H, halo, OH, CF3, alkyl, fluoroalkyl, alkoxy, Ph, amino, certain heterocyclyl, etc.; R3 = (un) substituted Ph; R4 = (un) substituted alkyl, alkenyl, cycloalkylmethyl, or heterocyclylalkyl]. The compds. are useful as hypocholesterolemic agents, hypotriglyceridemic agents, antiatherosclerosis agents, antifungal agents, anti-Alzheimer's agents, and anti-acne agents (no data). Examples include over 200 invention compds. For instance, reductive alkylation of 4-ClC6H4NH2 with pivaldehyde and NaBH4 gave 99% 4-ClC6H4NHCH2CMe3, which reacted with BC13 and then 2,3-ethylenedioxybenzaldehyde and Et3N to give 88% (5-chloro-2-neopentylaminophenyl)(2,3-ethylenedioxyphenyl)methanol. The latter underwent a sequence of amidation with (E)-ClCOCH:CHCO2Et (90%), cyclization by treatment with K2CO3 in EtOH (67%), alkaline saponification of

ΙI

the ester (91%), and amidation with Et isonipecotate (68%), to give title compound II.

IT 201218-86-2P 201218-89-5P 201218-92-0P 201218-95-3P 201219-01-4P 201219-06-9P 201219-13-8P 201219-14-9P 201219-28-5P 201219-36-5P 201219-37-6P 201219-74-1P 201219-75-2P 201219-86-5P 201219-87-6P 201219-89-8P 201219-90-1P 201220-01-1P 201220-06-6P 201220-07-7P 201220-21-5P 201220-29-3P 201220-30-6P 201220-71-5P 201220-72-6P 201419-55-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzoxazepines and benzothiazepines as squalene synthetase inhibitors)

RN 201218-86-2 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 201218-89-5 CAPLUS

CN 3-Piperidinecarboxylic acid, $1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester, <math>(3\alpha,5\beta)-[partial]-(9CI)$ (CA INDEX NAME)

Relative stereochemistry.

RN 201218-92-0 CAPLUS

CN L-Proline, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 201218-95-3 CAPLUS

CN 2,4-Piperidinedicarboxylic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, dimethyl ester, $(3\alpha,5\beta)$ -[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 201219-01-4 CAPLUS

CN 2-Piperidinecarboxylic acid, $1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester, <math>(3\alpha,5\beta)-[partial]-(9CI)$ (CA INDEX NAME)

RN 201219-06-9 CAPLUS

CN 3-Piperidinecarboxylic acid, $1-[[7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-5-(2,3,4-trimethoxyphenyl)-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester, <math>(3\alpha,5\beta)-[partial]-(9CI)$ (CA INDEX NAME)

Relative stereochemistry.

RN 201219-13-8 CAPLUS

CN L-Proline, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

RN 201219-14-9 CAPLUS

CN D-Proline, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 201219-28-5 CAPLUS

CN 3-Azetidinecarboxylic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester, trans- (9CI) (CA INDEX NAME)

RN 201219-36-5 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[7-chloro-1-(cyclopropylmethyl)-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 201219-37-6 CAPLUS

CN 3-Piperidinecarboxylic acid, 1-[[7-chloro-1-(cyclopropylmethyl)-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester, $(3\alpha,5\beta)$ -[partial]- (9CI) (CA INDEX NAME)

RN 201219-74-1 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-9-fluoro-1,2,3,5-tetrahydro-7-methyl-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 201219-75-2 CAPLUS

CN 3-Piperidinecarboxylic acid, 1-[[5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-9-fluoro-1,2,3,5-tetrahydro-7-methyl-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester, (3α,5β)-[partial]-(9CI) (CA INDEX NAME)

RN 201219-86-5 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 201219-87-6 CAPLUS

CN 3-Piperidinecarboxylic acid, $1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, <math>(3\alpha,5\beta)-[partial]-(9CI)$ (CA INDEX NAME)

RN 201219-89-8 CAPLUS

CN L-Proline, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 201219-90-1 CAPLUS

CN 2,4-Piperidinedicarboxylic acid, $1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, <math>(3\alpha,5\beta)$ -[partial]- (9CI) (CA INDEX NAME)

RN 201220-01-1 CAPLUS

CN 3-Piperidinecarboxylic acid, 1-[[7-chloro-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-5-(2,3,4-trimethoxyphenyl)-4,1-benzoxazepin-3-yl]acetyl]-, $(3\alpha,5\beta)$ -[partial]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 201220-06-6 CAPLUS

CN L-Proline, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, (4R)-(9CI) (CA INDEX NAME)

RN 201220-07-7 CAPLUS

CN D-Proline, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, (4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 201220-21-5 CAPLUS

CN 3-Azetidinecarboxylic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, trans- (9CI) (CA INDEX NAME)

RN 201220-29-3 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[7-chloro-1-(cyclopropylmethyl)-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 201220-30-6 CAPLUS

CN 3-Piperidinecarboxylic acid, 1-[[7-chloro-1-(cyclopropylmethyl)-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, $(3\alpha,5\beta)$ -[partial]- (9CI) (CA INDEX NAME)

RN 201220-71-5 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-9-fluoro-1,2,3,5-tetrahydro-7-methyl-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 201220-72-6 CAPLUS

CN 3-Piperidinecarboxylic acid, $1-[[5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-9-fluoro-1,2,3,5-tetrahydro-7-methyl-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, <math>(3\alpha,5\beta)$ -[partial]- (9CI) (CA INDEX NAME)

$$MeO$$
 MeO
 MeO
 MeO
 R
 R
 F
 CMe_3

RN 201419-55-8 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, trans-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

IT 152909-46-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of benzoxazepines and benzothiazepines as squalene synthetase inhibitors)

RN 152909-46-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

10/2/56,198

ANSWER 22 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:365842 CAPLUS

DOCUMENT NUMBER: 127:34256

TITLE: Preparation of fused ring compounds as cholesterol

lowing agents

INVENTOR(S): Yukimasa, Hidefumi; Suqiyama, Yasuo; Tozawa, Ryuichi

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 19 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
							
	JP 09087260	A2	19970331	JP 1995-249758	19950927		
	PRIORITY APPLN. INFO.:			JP 1995-249758	19950927		
(OTHER SOURCE(S):	MARPAT	127:34256				
(GI						

$$\begin{array}{c|c}
R^2 \\
\downarrow \\
D \\
\downarrow \\
N \\
\downarrow \\
R^1
\end{array}$$
I

AB The title compds. [I; Rl = H, (un)substituted hydrocarbyl; R2 = H, (un)substituted hydrocarbyl, heterocyclyl; X = (un)substituted sulfonic acid, etc.; ring A = (un)substituted benzene ring or heterocycle ring; ring J = 7-8 numbered heterocycle; D = C, N; n = 1-2] are prepared I, possessing cholesterol, lipid, and triglyceride lowing activity, are useful for prevention and treatment of hyperlipemia. Thus, benzoxazepine derivative (II; X = Et) (preparation given) was treated with concentrate HCl in dioxane

to give the title compound II (X = H) (III). III which showed IC50 of 23 and 19 μM against rat and human cholesterol synthase resp. A capsule, tablet, and injectable formulation containing I were also prepared

IT 189681-29-6P 189681-31-0P 189681-33-2P 189681-34-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(Preparation of fused ring compds. as cholesterol lowing agents) 189681-29-6 CAPLUS

Phosphonic acid, [2-[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-, diethyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

RN

CN

Absolute stereochemistry.

RN 189681-31-0 CAPLUS

CN Phosphonic acid, [[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, diethyl ester, (3S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189681-33-2 CAPLUS

CN 4,1-Benzoxazepine-3-methanesulfonic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, sodium salt, (3S-trans)-(9CI) (CA INDEX NAME)

Na

RN 189681-34-3 CAPLUS

CN 4,1-Benzoxazepine-3-methanesulfonic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 189681-30-9P 189681-32-1P 189681-35-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(Preparation of fused ring compds. as cholesterol lowing agents)

RN 189681-30-9 CAPLUS

CN Phosphonic acid, [2-[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]ethyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189681-32-1 CAPLUS

CN Phosphonic acid, [[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, (3S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189681-35-4 CAPLUS

CN 4,1-Benzoxazepine-3-methanesulfonamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3S-trans)-(9CI) (CA INDEX NAME)

IT 171868-39-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(Preparation of fused ring compds. as cholesterol lowing agents)

RN 171868-39-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 189681-36-5P 189681-37-6P 189681-38-7P 189681-39-8P 189681-40-1P 189681-41-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(Preparation of fused ring compds. as cholesterol lowing agents)

RN 189681-36-5 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,5-dihydro-3-(2-hydroxyethyl)-, sodium salt, (3R-trans)-(9CI) (CA INDEX NAME)

Na

RN 189681-37-6 CAPLUS
CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,5-dihydro-3-[2-[(methylsulfonyl)oxy]ethyl]-, (3R-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189681-38-7 CAPLUS
CN 4,1-Benzoxazepin-2(3H)-one, 3-(aminomethyl)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,5-dihydro-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189681-39-8 CAPLUS

CN Thiocyanic acid, [7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]methyl ester, (3S-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189681-40-1 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,5-dihydro-3-(hydroxymethyl)-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189681-41-2 CAPLUS
CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,5-dihydro-3-[[(methylsulfonyl)oxy]methyl]-, (3R-trans)-(9CI) (CA INDEX NAME)

ANSWER 23 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:317788 CAPLUS

DOCUMENT NUMBER: 126:293368

TITLE: Benzoxazepine compounds, their production and use as

lipid lowering agents

Yukimasa, Hidefumi; Sugiyama, Yasuo; Tozawa, Ryuichi INVENTOR(S): PATENT ASSIGNEE(S):

Takeda Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 112 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA?	PATENT NO.				KIND DATE		APPLICATION NO.						DATE				
WO						WO 1996-JP2596						19960912					
	W:	AL,	AM.	AU,	AZ.	BA.	BB.	BG.	BR.	. By	, CA,	CN.	CU.	CZ.	EE	. GE.	HU,
											LV,						
								-			I, TR,	-					
							RU,				-,,	,		•	-	•	•
	RW:										, DE,	DK.	ES.	FI.	FR	. GB.	GR.
											CF,						
					TD,		,	,	,		,,	/	,	,		,,	,
CA	2231	-			AA		1997	0320		CA	1996-	2231	052			19960	912
AU	9669	442			A1		1997	0401		ΑU	1996-	6944	2			19960	912
JP	0913	6880			A2		1997	0527		JP	1996-	2423	78			19960	912
JP	3479	796			В2		2003	1215									
EP	8625	62			A1		1998	0909		ΕP	1996- 1996-	9303	65			19960	912
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	, GF	R, IT,	LI,	LU,	NL,	SE	, MC,	PT,
		IE.	FI														
CN	1196	052			Α		1998	1014		CN	1996- 2000- 2000-	1968	92			19960	912
CN	1072	649			В		2001	1010									
JP	2001	0979	63		A2		2001	0410		JP	2000-	3233	10			19960	912
EP	1097	928			A1		2001	0509		ΕP	2000-	1266	72			19960	912
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	, GF	R, IT,	LI,	LU,	NL,	SE	, MC,	PT,
		IE,	FI														
AT	2027 2158 8625 9702	74			E		2001	0715		ΑT	1996-	9303	65			19960	
ES	2158	344			Т3		2001	0901		ES	1996- 1996- 1997-	9303	65			19960 19960	912
PT	8625	62			${f T}$		2001	1130		PT	1996-	9303	65			19960	912
ZA	9702	134			A		1999	0604		ZA	1997-	2134				19970	312
US	6110	909			Α		2000	0829		US	1998-	4326	5			19980	312
US	6613	761			В1					US	2000-	5879	47			20000	606
GR	3036 2004	707			Т3		2001	1231		GR	2001- 2003- 1995-	4015	64			20010	926
US	2004	0728	19		A1		2004	0415		US	2003-	6061	52			20030	624
RIORIT	Y APP	LN.	INFO	. :						JΡ	1995-	2354	57		A	19950	913
										ΕP	1996-	9303	65		A 3	19960	912
											1996-						
										WO	1996-	JP25	96	1	W	19960	912
										ZA	1997-	2134			A	19970	312
										US	1998-	4326	5		A 3	19980	312
										US	1997- 1998- 2000-	5879	47		A1	20000	606
THER SO	OURCE	(S):			MAR	TAS	126:	2933	68								

$$OR1$$
 $OR1$
 $OR1$

AB New benzoxazepines I [R = alkyl, hydroxyalkyl; R1 = alkyl; R2 = halogen; R3 = (un)substituted CONH2, heterocyclic group having a deprotonatable hydrogen atom]were prepared for use as cholesterol and triglyceride lowering agent. Thus, I [R = CH2CMe3, R1 = Me, R2 = Cl, R3 = CO2H] was amidated, dehydrated to the nitrile, and cyclized with Me3SiN3 to give I [R = CH2CMe3, R1 = Me, R2 = Cl, R3 = 5-tetrazolyl] which had a squalene synthetase inhibiting IC50 of 11X10-9 M.

IT 189058-78-4P 189059-51-6P 189059-84-5P 189059-85-6P 189059-92-5P

Ι

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of arylbenzoxazepinones as hypolipemic agents)

RN 189058-78-4 CAPLUS

CN 4-Piperidineacetic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-51-6 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,5-dihydro-3-(1H-tetrazol-5-ylmethyl)-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-84-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-N-(methylsulfonyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-85-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[3-hydroxy-2-(hydroxymethyl)-2-methylpropyl]-N-(methylsulfonyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189059-92-5 CAPLUS

CN Phosphonic acid, [[1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-piperidinyl]methyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

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IT
     189058-84-2P 189058-85-3P 189058-86-4P
     189058-88-6P 189058-91-1P 189058-94-4P
     189058-95-5P 189058-96-6P 189058-97-7P
     189059-02-7P 189059-05-0P 189059-06-1P
     189059-07-2P 189059-54-9P 189059-55-0P
     189059-72-1P 189059-79-8P 189059-80-1P
     189059-81-2P 189059-82-3P 189059-83-4P
     189059-90-3P 189059-91-4P 189059-93-6P
     189059-96-9P 189059-98-1P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of arylbenzoxazepinones as hypolipemic agents)
RN
     189058-84-2 CAPLUS
CN
     D-Isoleucine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethoxyphenyl)]
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dimethylpropy1)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-85-3 CAPLUS

CN L-Glutamic acid, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, 5-ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-86-4 CAPLUS

CN L-Aspartic acid, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

RN 189058-88-6 CAPLUS
CN Glycine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-91-1 CAPLUS
CN L-Phenylalanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

RN 189058-94-4 CAPLUS

CN Acetic acid, [1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-piperidinylidene]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-95-5 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189058-96-6 CAPLUS

CN 4-Piperidineacetic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-97-7 CAPLUS

CN β-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

RN 189059-02-7 CAPLUS

CN L-Tyrosine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-05-0 CAPLUS

CN L-Valine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

RN 189059-06-1 CAPLUS

CN L-Leucine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-07-2 CAPLUS

CN 1-Piperazineacetic acid, 4-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-54-9 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-3-[(2,5-dihydro-5-oxo-1,2,4-oxadiazol-3-yl)methyl]-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,5-dihydro-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-55-0 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,5-dihydro-3-(1H-tetrazol-5-ylmethyl)-, monosodium salt, (3R-trans)- (9CI) (CA INDEX NAME)

Na

RN 189059-72-1 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-79-8 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-[(2-methylphenyl)sulfonyl]-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-80-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-N-(phenylsulfonyl)-, (3R-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-81-2 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-[(1-methylethyl)sulfonyl]-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-82-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-N-(ethylsulfonyl)-1,2,3,5-tetrahydro-2-oxo-, (3R-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-83-4 CAPLUS

CN 4-Piperidinecarboxamide, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-N-(methylsulfonyl)-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-90-3 CAPLUS

CN 4-Piperidineacetamide, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-N-(methylsulfonyl)-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-91-4 CAPLUS

CN Phosphonic acid, [[[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-93-6 CAPLUS

CN Piperidine, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-(1H-tetrazol-5-ylmethyl)-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-96-9 CAPLUS

CN Piperidine, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-[2-(1H-tetrazol-5-yl)ethyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-98-1 CAPLUS

CN Phosphonic acid, [[[[7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 171868-39-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of arylbenzoxazepinones as hypolipemic agents)

RN 171868-39-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

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IT
     189058-37-5P 189058-38-6P 189058-39-7P
     189058-40-0P 189058-41-1P 189058-42-2P
     189058-43-3P 189058-44-4P 189058-45-5P
     189058-46-6P 189058-47-7P 189058-48-8P
     189058-49-9P 189058-50-2P 189058-51-3P
     189058-52-4P 189058-53-5P 189058-54-6P
     189058-55-7P 189058-56-8P 189058-57-9P
     189058-58-0P 189058-59-1P 189058-61-5P
     189058-62-6P 189058-63-7P 189058-64-8P
     189058-65-9P 189058-66-0P 189058-67-1P
     189058-68-2P 189058-69-3P 189058-70-6P
     189058-71-7P 189058-72-8P 189058-73-9P
     189058-74-0P 189058-75-1P 189058-76-2P
     189059-10-7P 189059-40-3P 189059-42-5P
     189059-52-7P 189059-53-8P 189059-57-2P
     189059-61-8P 189059-62-9P 189059-63-0P
     189059-64-1P 189059-65-2P 189059-66-3P
     189059-67-4P 189059-68-5P 189059-69-6P
     189059-71-0P 189059-87-8P 189059-88-9P
     189059-89-0P 189059-94-7P 189059-95-8P
     189059-97-0P 189060-00-2P 189060-01-3P
     189060-02-4P 189060-19-3P 189060-21-7P
     189060-24-0P 189060-27-3P 189060-30-8P
     189060-41-1P 189060-51-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of arylbenzoxazepinones as hypolipemic agents)
RN
     189058-37-5 CAPLUS
     1-Piperazineacetic acid, 4-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-
CN
     dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-,
     ethyl ester, (3R-trans)- (9CI) (CA INDEX NAME)
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RN 189058-38-6 CAPLUS

CN 4-Piperidineacetic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-39-7 CAPLUS

CN Glycine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 189058-40-0 CAPLUS

CN D-Serine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-41-1 CAPLUS

CN D-Threonine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 189058-42-2 CAPLUS

CN L-Proline, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-43-3 CAPLUS

CN L-Proline, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, methyl ester, (4R)- (9CI) (CA INDEX NAME)

RN 189058-44-4 CAPLUS

CN D-Isoleucine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-45-5 CAPLUS

CN L-Glutamic acid, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, 5-ethyl 1-methyl ester (9CI) (CA INDEX NAME)

RN 189058-46-6 CAPLUS

CN L-Aspartic acid, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-47-7 CAPLUS

CN L-Methionine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 189058-48-8 CAPLUS

CN Glycine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-49-9 CAPLUS

CN L-Serine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 189058-50-2 CAPLUS

CN L-Asparagine, N2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-51-3 CAPLUS

CN L-Phenylalanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN189058-52-4 CAPLUS

L-Glutamine, N2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-CN dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & \text{Me3C} \\ & \text{MeO} \\ & \text{O} \\ & \text{N} \\ & \text{O} \\ & \text{MeO} \\ & \text{OMe} \\ \end{array}$$

RN 189058-53-5 CAPLUS

CN L-Threonine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethoxyphenyl)]dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 189058-54-6 CAPLUS

CN Acetic acid, [1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-piperidinylidene]-, methyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-55-7 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, methyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189058-56-8 CAPLUS

CN 4-Piperidineacetic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, methyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-57-9 CAPLUS

CN β-Alanine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 189058-58-0 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, methyl ester, [3R-[trans(trans)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-59-1 CAPLUS

CN Cyclohexanecarboxylic acid, 1-[[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189058-61-5 CAPLUS

CN Benzeneacetic acid, 4-[[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, methyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-62-6 CAPLUS

CN L-Tyrosine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

RN

189058-63-7 CAPLUS L-Histidine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-CN dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

189058-64-8 CAPLUS RN

CN L-Tryptophan, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethoxyphenyl)]dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 189058-65-9 CAPLUS

CN L-Valine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-66-0 CAPLUS

CN L-Leucine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 189058-67-1 CAPLUS

CN 1-Piperazineacetic acid, 4-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-2-oxo-, 1,1-dimethylethyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-68-2 CAPLUS

CN 4-Piperidinepentanoic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189058-69-3 CAPLUS

CN 4-Piperidinebutanoic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-70-6 CAPLUS

CN 2-Butenoic acid, $4-[1-[(7-\text{chloro}-5-(2,3-\text{dimethoxyphenyl})-1-(2,2-\text{dimethylpropyl})-1,2,3,5-\text{tetrahydro}-2-\text{oxo}-4,1-\text{benzoxazepin}-3-yl]acetyl]-4-piperidinyl]-, ethyl ester, <math>[3R-[3\alpha(E),5\beta]]-(9CI)$ (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 189058-71-7 CAPLUS

CN 4-Piperidineacetic acid, 4-(acetyloxy)-1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-72-8 CAPLUS

CN 4-Piperidinepropanoic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189058-73-9 CAPLUS

CN Phosphonic acid, [[1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-piperidinyl]methyl]-, bis(1-methylethyl) ester, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-74-0 CAPLUS

CN Phosphonic acid, [[[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, diethyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189058-75-1 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-76-2 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-10-7 CAPLUS

CN 4-Piperidinepropanoic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-40-3 CAPLUS

CN 4-Piperidinecarbonitrile, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-42-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-N-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propyl]-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-52-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189059-53-8 CAPLUS

CN 4,1-Benzoxazepine-3-acetonitrile, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-57-2 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-1-(3-hydroxy-2,2-dimethylpropyl)-3-(1H-tetrazol-5-ylmethyl)-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189059-61-8 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-, ethyl ester, (3R,5S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-62-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-N-(3-cyanopropyl)-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-63-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-N-(3-cyanopropyl)-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-64-1 CAPLUS

CN 1H-Tetrazole-1-propanenitrile, 5-[[7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]methyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-65-2 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-66-3 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 189059-67-4 CAPLUS

CN Acetic acid, [1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-piperidinylidene]-, methyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-68-5 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, methyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-69-6 CAPLUS

CN 4-Piperidineacetic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, methyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-71-0 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 189059-87-8 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-1-[(2,2,5-trimethyl-1,3-dioxan-5-yl)methyl]-, ethyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-88-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[3-hydroxy-2-(hydroxymethyl)-2-methylpropyl]-2-oxo-, ethyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-89-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-1-[(2,2,5-trimethyl-1,3-dioxan-5-yl)methyl]-, (3R-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-94-7 CAPLUS

CN 4-Piperidineacetamide, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-95-8 CAPLUS

CN 4-Piperidineacetonitrile, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-97-0 CAPLUS

CN Phosphonic acid, [[[[7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, diethyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189060-00-2 CAPLUS

CN 4-Piperidineacetic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-1-[(2,2,5-trimethyl-1,3-dioxan-5-yl)methyl]-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

`Absolute stereochemistry.

RN 189060-01-3 CAPLUS

CN 4-Piperidineacetic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[3-hydroxy-2-(hydroxymethyl)-2-methylpropyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189060-02-4 CAPLUS

CN 4-Piperidineacetic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[3-hydroxy-2-(hydroxymethyl)-2-methylpropyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-19-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[3-hydroxy-2-(hydroxymethyl)-2-methylpropyl]-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189060-21-7 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-1-[3-hydroxy-2-(hydroxymethyl)-2-methylpropyl]-3-(1H-tetrazol-5-ylmethyl)-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-24-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-1-[(2,2,5-trimethyl-1,3-dioxan-5-yl)methyl]-, (3R-trans)-(9CI) (CA INDEX NAME)

RN 189060-27-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetonitrile, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-1-[(2,2,5-trimethyl-1,3-dioxan-5-yl)methyl]-, (3R-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-30-8 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-3-(1H-tetrazol-5-ylmethyl)-1-[(2,2,5-trimethyl-1,3-dioxan-5-yl)methyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189060-41-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-N-[2-(1-pyrrolidinyl)ethyl]-1-[(2,2,5-trimethyl-1,3-dioxan-5-yl)methyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-51-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

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IT
     189058-77-3P 189058-79-5P 189058-80-8P
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     189058-87-5P 189058-89-7P 189058-90-0P
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     189060-37-5P 189060-45-5P 189060-48-8P
     RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
     study); PREP (Preparation); USES (Uses)
        (preparation of arylbenzoxazepinones as hypolipemic agents)
RN
     189058-77-3 CAPLUS
     1-Piperazineacetic acid, 4-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-
CN
     dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-,
     (3R-trans) - (9CI) (CA INDEX NAME)
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RN 189058-79-5 CAPLUS

CN Glycine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-80-8 CAPLUS

CN D-Serine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

RN 189058-81-9 CAPLUS

CN D-Threonine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-82-0 CAPLUS

CN L-Proline, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

RN 189058-83-1 CAPLUS

CN L-Proline, 1-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-87-5 CAPLUS

CN L-Methionine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

RN 189058-89-7 CAPLUS

CN L-Serine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-90-0 CAPLUS

CN L-Asparagine, N2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & &$$

RN 189058-92-2 CAPLUS

CN L-Glutamine, N2-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 189058-93-3 CAPLUS

CN L-Threonine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

RN 189058-98-8 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[[[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]methyl]-, [3R-[trans(trans)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189058-99-9 CAPLUS

CN Cyclohexanecarboxylic acid, 1-[[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-01-6 CAPLUS

CN Benzeneacetic acid, 4-[[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]amino]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-03-8 CAPLUS

CN L-Histidine, N-[[(3R,5S)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

RN 189059-04-9 CAPLUS

CN L-Tryptophan, N-[[(3R,5s)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-08-3 CAPLUS

CN 4-Piperidinepentanoic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

$$MeO$$
 MeO
 MeO
 R
 R
 CMe_3

RN 189059-09-4 CAPLUS

CN 4-Piperidinebutanoic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$MeO$$
 MeO
 R
 R
 $C1$
 R
 R
 $CMe3$

RN 189059-11-8 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, N-(3-aminopropyl)-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, monohydrochloride, (3R-trans)- (9CI) (CA INDEX NAME)

$$Me3C$$
 $(CH_2)_3$
 N
 H_2N
 $(CH_2)_3$
 N
 MeO
 OMe

HC1

RN 189059-12-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-[2-(4-morpholinyl)ethyl]-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-13-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-N-[2-(1-piperidinyl)ethyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-14-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-N-[3-(1-piperidinyl)propyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-15-2 CAPLUS

CN 1,4'-Bipiperidine, 1'-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, monohydrochloride, (3R-trans)- (9CI) (CA INDEX NAME)

● HCl

RN 189059-16-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-N-[[4-(dimethylamino)phenyl]methyl]-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-17-4 CAPLUS

CN 4-Piperidinamine, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-N,N-dimethyl-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-18-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-N-[3-(3,4-dihydro-2(1H)-isoquinolinyl)propyl]-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-19-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-N-[2-(1-pyrrolidinyl)ethyl]-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189059-20-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-[3-(4-morpholinyl)propyl]-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-21-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-N-[3-(1-pyrrolidinyl)propyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-22-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-N-(2-pyridinylmethyl)-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-23-2 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-[3-(1H-imidazol-1-yl)propyl]-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-24-3 CAPLUS

CN 4-Piperidinol, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 189059-25-4 CAPLUS

CN 2-Pyrrolidinemethanol, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, [3R-[3 α (R*),5 β]]- (9CI) (CA INDEX NAME)

RN 189059-26-5 CAPLUS

CN 2-Pyrrolidinemethanol, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, [3R-[3 α (S*),5 β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-27-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-[1-(hydroxymethyl)-3-methylbutyl]-2-oxo-, $[3R-[3\alpha(R^*),5\beta]]$ - (9CI) (CA INDEX NAME)

RN 189059-28-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-[1-(hydroxymethyl)-3-methylbutyl]-2-oxo-, $[3R-[3\alpha(S^*),5\beta]]$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-29-8 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-(2-hydroxy-1-phenylethyl)-2-oxo-, [3R-[3 α (R*),5 β]]- (9CI) (CA INDEX NAME)

RN 189059-30-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-[1-(hydroxymethyl)-2-methylpropyl]-2-oxo-, $[3R-[3\alpha(S^*),5\beta]]$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-31-2 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-[2-hydroxy-1-(hydroxymethyl)ethyl]-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-32-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-(3-hydroxypropyl)-2-oxo-, (3R-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-33-4 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-(2-hydroxyethyl)-2-oxo-, (3R-trans)-(9CI) (CA INDEX NAME)

RN 189059-34-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-[1-(hydroxymethyl)-2-phenylethyl]-2-oxo-, $[3R-[3\alpha(S^*),5\beta]]$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-35-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-(2-hydroxy-1-methylethyl)-2-oxo-, [$3R-[3\alpha(R^*),5\beta]$]- (9CI) (CA INDEX NAME)

RN 189059-36-7 CAPLUS

CN Piperidine, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4,4-dimethoxy-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-37-8 CAPLUS

CN 1,4-Dioxa-8-azaspiro[4.5]decane, 8-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-38-9 CAPLUS

CN 4-Piperidinone, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-39-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, N-[[4-(aminosulfonyl)phenyl]methyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \\ \text{MeO} \\ \text{MeO} \\ \text{N} \\ \text{N} \\ \text{CMe} \\ \text{S} \\ \text{O} \\ \text$$

RN 189059-41-4 CAPLUS

CN 4-Piperidinecarboxamide, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-43-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-[2-methyl-6-(1-methylethyl)phenyl]-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-44-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-N-(2,4-difluorophenyl)-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-45-8 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-N-2-propenyl-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-46-9 CAPLUS

CN Morpholine, 4-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-47-0 CAPLUS

CN Piperidine, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI)
(CA INDEX NAME)

RN 189059-48-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N,N-dimethyl-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-49-2 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-N-(1H-tetrazol-5-ylmethyl)-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-50-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-N-1H-tetrazol-5-yl-, (3R-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-56-1 CAPLUS

CN Piperidine, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-(1H-tetrazol-5-yl)-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-70-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-N-[2-(1-pyrrolidinyl)ethyl]-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-73-2 CAPLUS

CN Acetic acid, [1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-piperidinylidene]-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-74-3 CAPLUS

CN 4-Piperidinecarboxylic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-75-4 CAPLUS

CN 4-Piperidineacetic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(3-hydroxy-2,2-dimethylpropyl)-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-76-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-[(4-methylphenyl)sulfonyl]-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-77-6 CAPLUS

CN 4-Piperidineacetamide, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-N-(methylsulfonyl)-, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189059-78-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-N-(methylsulfonyl)-2-oxo-, (3R-trans)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189059-99-2 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, [[[1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-piperidinyl]methyl]phosphinylidene]bis(oxymethylene) ester, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189060-04-6 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2-[(acetyloxy)methyl]-2-methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-05-7 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2-[(acetyloxy)methyl]-2-methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

RN 189060-07-9 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 1-[3-(acetyloxy)-2-[(acetyloxy)methyl]-2-methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-N-(methylsulfonyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-10-4 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 189060-13-7 CAPLUS

CN 4-Piperidineacetic acid, 1-[[(3R,5S)-1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-16-0 CAPLUS

CN 4-Piperidineacetic acid, 1-[[7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[3-hydroxy-2-(hydroxymethyl)-2-methylpropyl]-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-4-hydroxy-, methyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

RN 189060-33-1 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2-[(acetyloxy)methyl]-2-methylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-3-(1H-tetrazol-5-ylmethyl)-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-37-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-[3-hydroxy-2-(hydroxymethyl)-2-methylpropyl]-2-oxo-N-[2-(1-pyrrolidinyl)ethyl]-, (3R,5S)- (9CI) (CA INDEX NAME)

RN 189060-45-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetamide, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-N-(methylsulfonyl)-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189060-48-8 CAPLUS

CN 4,1-Benzoxazepin-2(3H)-one, 1-[3-(acetyloxy)-2,2-dimethylpropyl]-7-chloro-5-(2,3-dimethoxyphenyl)-1,5-dihydro-3-(1H-tetrazol-5-ylmethyl)-, (3R,5S)-(9CI) (CA INDEX NAME)

10/256,198

ANSWER 24 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:457956 CAPLUS

DOCUMENT NUMBER: 125:123701

TITLE: Antihypertriglyceridemic composition
INVENTOR(S): Sugiyama, Yasuo; Yukimasa, Hidefumi
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Can. Pat. Appl., 59 pp.

CODEN: CPXXEB

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
				-	
CA 2160092	AA	19960408	CA 1995-2160092		19951006
PRIORITY APPLN. INFO.:			JP 1994-94	U	19941007

OTHER SOURCE(S): MARPAT 125:123701
GI For diagram(s), see printed CA Issue.

AB An antihypertriglyceridemic composition comprises a compound I (R1 = H, hydrocarbon group; R2, R3 = H, hydrocarbon, group, heterocyclic group; X = carboxyl group, carbamoyl group, OH, amino group, heterocyclic group; A = benzene ring, heterocyclic ring; J = 7- or 8-membered heterocyclic ring) or a pharmacol. acceptable salt thereof. The composition has a plasma triglyceride concentration-lowering activity, and therefore is useful for the prophylaxis or treatment of hypolipemia, such as hypertriglyceridemia. Examples for formulating capsules, tablets, and injections containing I are given.

IT 171868-39-6 171962-07-5 179124-62-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(hypolipemic compns. containing fused-cyclic compds.)

RN 171868-39-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 171962-07-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-

dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, sodium salt, (3R,5S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Na

RN 179124-62-0 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1,2,3,5-tetrahydro-1-(2-methylpropyl)-2-oxo-, (3R-trans)- (9CI) (CA INDEX NAME)

10/256, 198

ANSWER 25 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:342064 CAPLUS

DOCUMENT NUMBER: 125:32076

TITLE: Production of optically active compounds

INVENTOR(S): Nakahama, Kazuo; Izawa, Motowo; Nagano, Yoichi; Tarui, Naoki; Matsumoto, Kiyoharu; Kori, Masakuni; Kanamaru,

Tsuneo; Nagata, Toshiaki

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Eur. Pat. Appl., 54 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 710725	A1	19960508	EP 1995-117120	19951031
R: AT, BE, CH,	DE, DK	, ES, FR,	GB, GR, IE, IT, LI,	LU, MC, NL, PT, SE
JP 08205889	A2	19960813	JP 1995-281162	19951030
CA 2161849	AA	19960502	CA 1995-2161849	19951031
US 5770438	Α	19980623	US 1995-550643	19951031
JP 08298995	A2	19961119	JP 1996-47356	19960305
PRIORITY APPLN. INFO.:			JP 1994-269056	A 19941101
			JP 1995-47156	A 19950307
			EP 1995-117120	A 19951031

OTHER SOURCE(S): MARPAT 125:32076

GI For diagram(s), see printed CA Issue.

AB A process is claimed for producing optically active compds. of formula (I) that have plasma cholesterol- and triglyceride-lowering activities, wherein R1 represents H or a hydrocarbon group that may be substituted; R2 and R3 independently represent H, a hydrocarbon group that may be substituted, or a heteroarom. group that may be substituted; X1 represents a substituent comprising an esterified carboxyl group or an acylated OH group; ring A represents a benzene ring that may be substituted or a heteroarom. ring that may be substituted; ring J1 represents a 7- or 8-membered heterocyclic ring containing ≤3 hetero atoms, which may have a further substituent or substituents in addition to R1, R2, R3, and X1, and C1 denotes a chiral C atom or a salt thereof. The process comprises subjecting the racemic compound of the formula I or a salt thereof, or alternatively a racemic starting compound for synthesizing the compound of the formula I to enzymically enantioselective hydrolysis to provide an optically active form thereof.

IT 177567-40-7P

RL: BPN (Biosynthetic preparation); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(optically active hypolipemic heterocyclic compound production involving biol. resolution)

RN 177567-40-7 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester, (3R,5S)- (9CI) (CA INDEX NAME)

IT 152909-22-3P

RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)

(optically active hypolipemic heterocyclic compound production involving biol. resolution of)

RN 152909-22-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

10/256,198

ANSWER 26 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:298262 CAPLUS

DOCUMENT NUMBER: 125:19089

TITLE: Pharmaceutical compositions containing condensed

seven- or eight-membered heterocyclic compounds useful

as antihypertriglyceridemic agents Sugiyama, Yasuo; Yukimasa, Hidefumi

INVENTOR(S): Sugiyama, Yasuo; Yukimasa, Hidefumi
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Eur. Pat. Appl., 26 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE			
EP 705607	A2	19960410	EP 1995-115109	19950926			
EP 705607	A3	19960508					
R: AT, BE, CH,	DE, DK	, ES, FR, GB	, GR, IE, IT, LI, LU,	NL, PT, SE			
TW 401301	В	20000811	TW 1995-84109892	19950921			
JP 08157369	A2	19960618	JP 1995-256283	19951003			
NO 9503961	Α	19960409	NO 1995-3961	19951005			
NO 308580	B1	20001002					
AU 9533081	A1	19960418	AU 1995-33081	19951005			
AU 703422	B2	19990325					
ни 73422	A2	19960729	HU 1995-2918	19951005			
FI 9504773	Α	19960408	FI 1995-4773	19951006			
CN 1128657	Α	19960814	CN 1995-117761	19951006			
RU 2166320	C2	20010510	RU 1995-117068	19951006			
PRIORITY APPLN. INFO.:			JP 1994-244136	A 19941007			

OTHER SOURCE(S): MARPAT 125:19089

GI For diagram(s), see printed CA Issue.

AB An antihypertriglyceridemic composition comprises condensed seven— or eight-membered heterocyclic compds. (I; R1 = H, hydrocarbyl; R2, R3 = H, hydrocarbyl, X' = a carboxyl that may be esterified, a carbamoyl that may be substituted, a hydroxyl that may be substituted, an amino that may be substituted, or an optionally substituted heterocyclic group having a hydrogen atom that may be deprotonated; ring A = represents a benzene ring that may be substituted or a heterocyclic ring that may be substituted; ring J' = a 7— or 8—membered heterocyclic ring having at most 3 hetero-atoms as ring constituent members; and ring J' may have a further substituent in addition to R1, R2 and X'), or a pharmacol. acceptable salt thereof. The composition has a plasma triglyceride concentration—lowering activity,

and therefore is useful for the prophylaxis or treatment of hyperlipemia, such as hypertriglyceridemia. A solution of sodium (3R, 5S)-7-chloro-5-(2,3-dimthyoxyphenyl)-1-neopentyl-2-oxo-,1,2,3,5-tetrahydro-4,1-benzoxazepine-3-acetate (II) in 0.5% methylcellulose was administered at 30 mg/kg/day to rats for 2 wk under non-fasted condition. The total plasma cholesterol was decreased from 186 to 160 mg/dL and the triglycerides decreased from 353 to 230 mg/dL. A capsule contained II 10, lactose 90, microcryst. cellulose 70, and magnesium stearate 10 mg.

IT 171868-39-6 171962-07-5

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(pharmaceutical compns. containing condensed seven- or eight-membered

heterocyclic compds. useful as antihypertriglyceridemic agents)

RN 171868-39-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 171962-07-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, sodium salt, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Na

L4 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:994196 CAPLUS

DOCUMENT NUMBER: 124:55994

TITLE: Optically active 4,1-benzoxazepine derivatives useful

as squalene synthase inhibitors

INVENTOR(S): Yukimasa, Hidefumi; Tozawa, Ryuichi; Kori, Masakuni;

Kitano, Kazuaki

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 41 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.					KIND DATE			APPLICATION NO.						DATE			
WO	WO 9521834			A1 19950817			WO 1995-JP148						19950206				
	W:	AM,	AU,	BB,	BG,	BR,	BY,	CA,	CN,	CZ	, EE,	FI,	GE,	HU,	KG,	KR,	KZ,
		LK,	LR,	LT,	LV,	MD,	MG,	MN,	MX,	NO	, NZ,	PL,	RO,	RU,	SI,	SK,	ТJ,
		TT,	UA,	UZ,	VN												
	RW:	KE,	MW,	SD,	SZ,	AT,	BE,	CH,	DE,	DK	, ES,	FR,	GB,	GR,	IE,	IT,	LU,
		MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI	, CM,	GA,	GN,	ML,	MR,	NE,	SN,
		TD,	TG														
RU	2170	732			C2		2001	0720	I	RU	1999-	1182	98		1	9930	419
AU	9515	898			A1		1995	0829	1	UΑ	1995-	1589	В		1	9950:	206
JP	0726	7939			A2		1995	1017	į.	JΡ	1995-	18972	2		1	9950:	207
BR	9501	469			Α		1997	0819	1	BR	1995-	L469			1	9950	406
PRIORIT	Y APP	LN.	INFO	.:					i	JΡ	1994-	1553	1	i	A 1	9940:	209
									7	OW	1995-	JP14	В	1	A 1	9950	206

OTHER SOURCE(S): MARPAT 124:55994

GΙ

AB Optically active 4,1-benzoxazepin-2-one derivs. I with (3R-trans)-configuration are disclosed [wherein R1 = alkyl; X = H or metal ion; ring A is substituted with halo; ring B is substituted with alkoxy]. I are useful for the prophylaxis or treatment of hypercholesteremia or coronary sclerosis in mammals. For example racemic trans-II was amidated with H-Ala-OBu-tert.HCl, and the resultant diastereomeric amides were separated by chromatog., deprotected, and hydrolyzed in acid and base, to give

both the desired isomer (3R,5S)-II (A) and its enantiomer (3S,5R)-II (B). In an assay for inhibition of human hepatic squalene synthase in vitro, isomer A had IC50 of 0.011 μ M, vs. 0.020 μ M for its 2-chlorophenyl analog [known from EP 567026]. In a rat enzyme system, the IC50 of isomer A was 0.026 μ M, whereas isomer B only gave 43% inhibition at 10-5 M.

IT 171868-39-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(desired stereoisomer; preparation of optically active 4,1-benzoxazepine derivs. as squalene synthase inhibitors)

RN 171868-39-6 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 171962-07-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(desired stereoisomer; preparation of optically active 4,1-benzoxazepine derivs. as squalene synthase inhibitors)

RN 171962-07-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, sodium salt, (3R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Na

TT 171768-62-0P 171768-63-1P 171868-45-4P 171868-46-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of optically active 4,1-benzoxazepine derivs. as squalene synthase inhibitors)

RN 171768-62-0 CAPLUS

CN L-Alanine, N-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, 1,1-dimethylethyl ester, (3S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 171768-63-1 CAPLUS

CN L-Alanine, N-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3S-trans)- (9CI)
(CA INDEX NAME)

RN 171868-45-4 CAPLUS

CN L-Alanine, N-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, 1,1-dimethylethyl ester, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 171868-46-5 CAPLUS

CN L-Alanine, N-[[7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)1,2,3,5-tetrahydro-2-oxo-4,1-benzoxazepin-3-yl]acetyl]-, (3R-trans)- (9CI)
(CA INDEX NAME)

IT 171868-38-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BYP (Byproduct); PUR (Purification or recovery); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(low-activity stereoisomer; preparation of optically active

4,1-benzoxazepine derivs. as squalene synthase inhibitors)

RN 171868-38-5 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 152909-46-1

RL: RCT (Reactant); RACT (Reactant or reagent) (starting material; preparation of optically active 4,1-benzoxazepine derivs. as squalene synthase inhibitors)

RN 152909-46-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

√44 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:164246 CAPLUS

DOCUMENT NUMBER: 120:164246

TITLE: 4,1-Benzoxazepines as squalene synthase inhibitors and

their use in the treatment of hypercholesteremia and

as fungicides

INVENTOR(S): Yukimasa, Hidefumi; Tozawa, Ryuichi; Kori, Masakuni;

Kitano, Kazuaki

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Eur. Pat. Appl., 194 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.			KIND DATE		APPLICATION NO.						DATE						
			A1 B1		19931027 20030326		EP 19		1993-106276			1	1993041				
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AT	2354	/4			E		2003	0415		AT	1993	-T06	276		1	9930	417
AU	93370	003			A1		1993	1021		ΑU	1993	-370)3		1	9930	419
AU	65954	13			B2		1995	0518									
CA	20943	335			AA		1993	1021		CA	1993	-209	1335		1	9930	419
CA	20943	335			С		1993	1021									
NO	93014	133			Α		1993	1021		NO	1993	-143	3		1	9930	419
ИО	30452	20			В1		1999	0104									
RU	21456	503			C1		2000	0220		RU	1993	-533	2		1	9930	419
CN	10834	181			Α		1994	0309		CN	1993	-106	358		1	9930	420
CN	10442	237			В		1999	0721									
JP	06239	9843			A2		1994	0830		JP	1993	-117	357		1	9930	420
JP	32836	528			B2		2002	0520									
HU	71482	2			A2		1995	1128		HU	1993	-116	1		1	9930	420
PRIORITY	APPI	LN.	INFO	. :						JΡ	1992	-995	11		A 1	9920	420
										JР	1992	-3399	947		A 1	9921	221

OTHER SOURCE(S): MARPAT 120:164246

GΙ

AB The titled compds. I [R1 = H, (un)substituted hydrocarbon group; R2, R3 = H, (un)substituted lower alkyl, (un)substituted Ph or aromatic heterocyclic group; X = direct bond, Z1-7 bridging group; Y = optionally esterified or thioesterified carboxyl group, (un)substituted OH, (un)substituted NH2, (un)substituted Ph, (un)substituted carbamoyl, etc.; ring A may be optionally substituted], which demonstrate inhibition of pathogenic fungal

growth and inhibition of the enzyme squalene synthetase, are prepared and I-containing formulations presented. Thus, the Et ester of N-[(3-R,5-S)-7-chloro-5-(2-chlorophenyl)-1-neopentyl-2-oxo-1,2,3,5-tetrahydro-4,1-benzoxazepine-3-acetyl]aminocetate was hydrolyzed in NaOH solution, producing N-[(3R,5S)-7-chloro-5-(2-chlorophenyl)-1-neopentyl-2-oxo-1,2,3,5-tetrazo-4,1-benzoxazepine-3-acetyl]aminoacetic acid (II). II demonstrated 50% inhibitory concentration against human squalene synthetase of 0.06 x 10-7 M.

IT 152909-22-3P 152909-46-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and squalene synthase inhibitory activity and fungicidal activity of)

RN 152909-22-3 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, ethyl ester, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 152909-46-1 CAPLUS

CN 4,1-Benzoxazepine-3-acetic acid, 7-chloro-5-(2,3-dimethoxyphenyl)-1-(2,2-dimethylpropyl)-1,2,3,5-tetrahydro-2-oxo-, (3R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.